



## wwPDB EM Validation Summary Report ⓘ

May 17, 2025 – 09:57 PM EDT

PDB ID : 8UA8 / pdb\_00008ua8  
EMDB ID : EMD-42054  
Title : Structure of Semliki Forest virus VLP in complex with VLDLR LA2  
Authors : Abraham, J.; Yang, P.; Li, W.; Fan, X.; Pan, J.  
Deposited on : 2023-09-20  
Resolution : 3.70 Å(reported)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

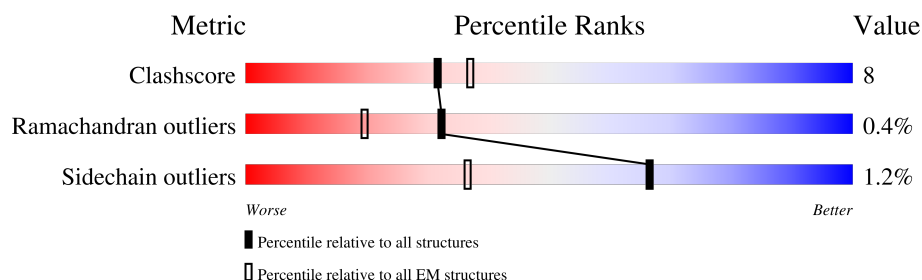
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	
1	E	438	
1	I	438	
1	M	438	
2	B	417	
2	F	417	
2	J	417	
2	N	417	

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Mol	Chain	Length	Quality of chain
3	C	54	
3	G	54	
3	K	54	
3	O	54	
4	D	153	
4	H	153	
4	L	153	
4	P	153	
5	R	37	
6	Q	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	a	2	
7	S	3	
7	T	3	
7	Y	3	
7	Z	3	
7	b	3	
7	c	3	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 33212 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	438	Total	C	N	O	S	0	0
			3329	2109	559	636	25		
1	E	438	Total	C	N	O	S	0	0
			3329	2109	559	636	25		
1	I	437	Total	C	N	O	S	0	0
			3318	2103	555	635	25		
1	M	437	Total	C	N	O	S	0	0
			3318	2103	555	635	25		

- Molecule 2 is a protein called Glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	417	Total	C	N	O	S	0	0
			3249	2052	576	596	25		
2	F	415	Total	C	N	O	S	0	0
			3234	2043	572	594	25		
2	J	417	Total	C	N	O	S	0	0
			3249	2052	576	596	25		
2	N	413	Total	C	N	O	S	0	0
			3218	2034	567	592	25		

- Molecule 3 is a protein called Assembly protein E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	51	Total	C	N	O	S	0	0
			392	246	63	75	8		
3	G	52	Total	C	N	O	S	0	0
			404	252	67	77	8		
3	K	51	Total	C	N	O	S	0	0
			392	246	63	75	8		
3	O	53	Total	C	N	O	S	0	0
			404	253	65	78	8		

- Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	152	Total	C	N	O	S	0	0
			1163	728	208	221	6		
4	H	153	Total	C	N	O	S	0	0
			1171	734	209	222	6		
4	L	153	Total	C	N	O	S	0	0
			1165	731	206	222	6		
4	P	153	Total	C	N	O	S	0	0
			1171	734	209	222	6		

- Molecule 5 is a protein called Very low-density lipoprotein receptor.

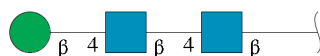
Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	37	Total	C	N	O	S	0	0
			275	158	46	65	6		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



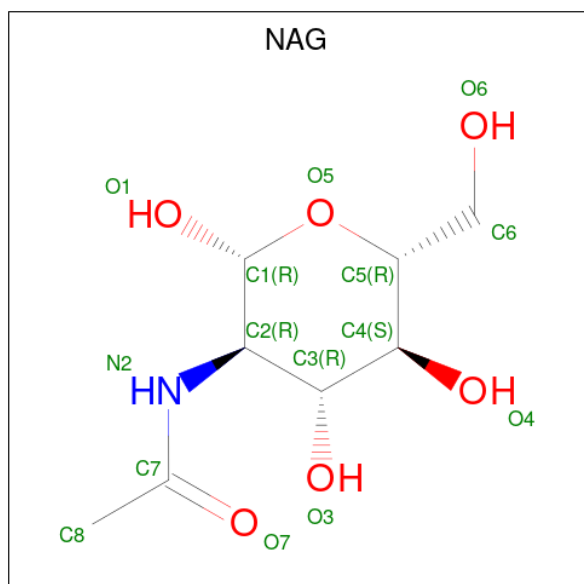
Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	3	Total	C	N	O	0	0
			39	22	2	15		
7	T	3	Total	C	N	O	0	0
			39	22	2	15		
7	Y	3	Total	C	N	O	0	0
			39	22	2	15		
7	Z	3	Total	C	N	O	0	0
			39	22	2	15		
7	b	3	Total	C	N	O	0	0
			39	22	2	15		
7	c	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	

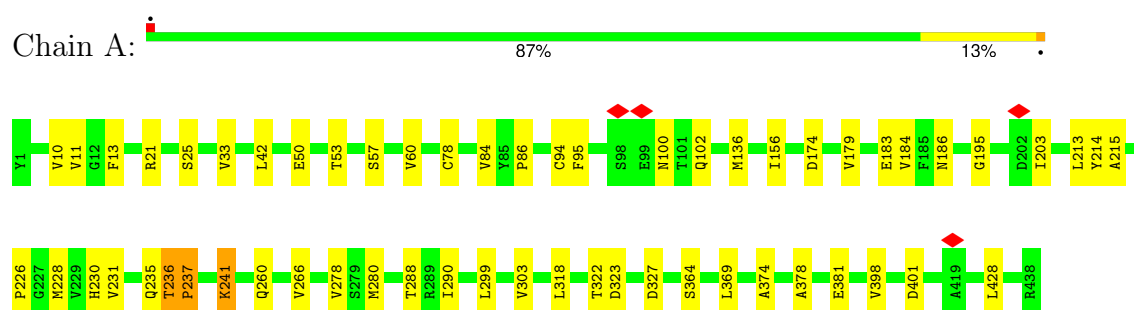
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	R	1	Total	Ca	0
			1	1	

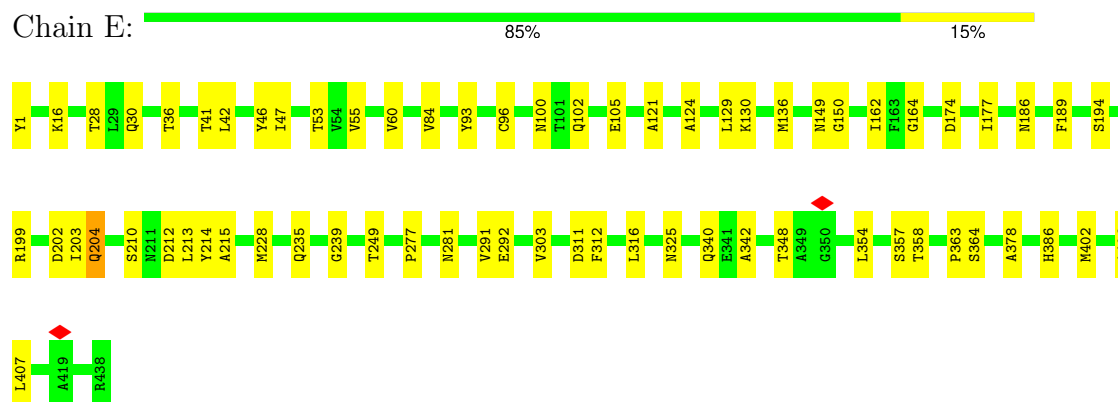
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

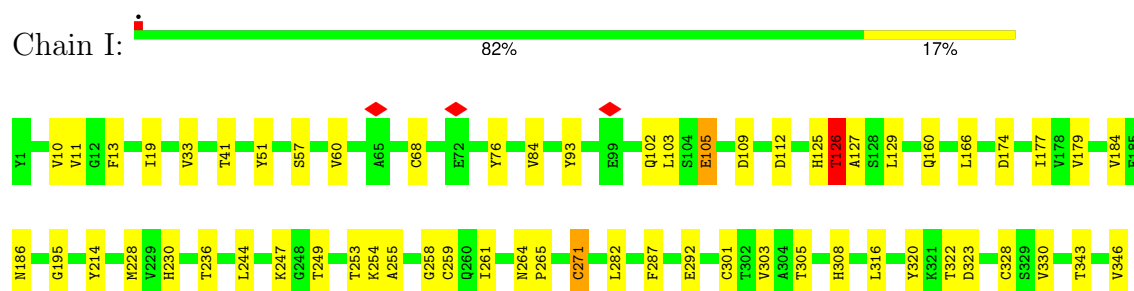
- Molecule 1: Glycoprotein E1

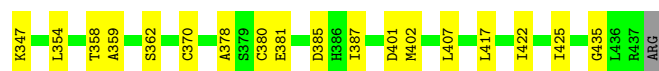


- Molecule 1: Glycoprotein E1

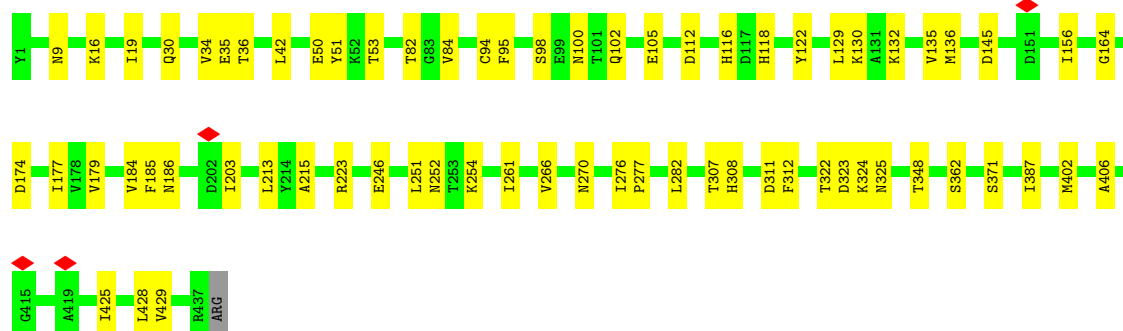
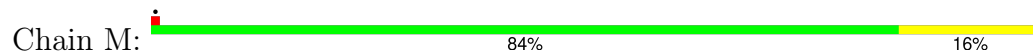


- Molecule 1: Glycoprotein E1

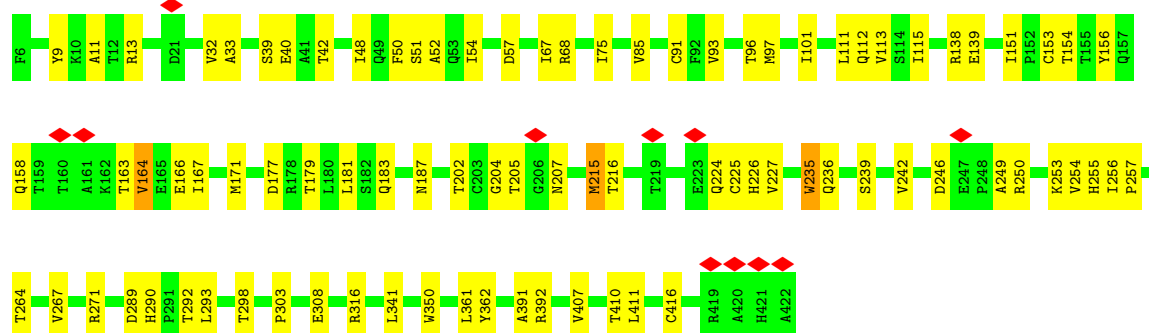
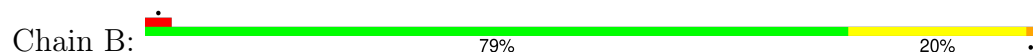




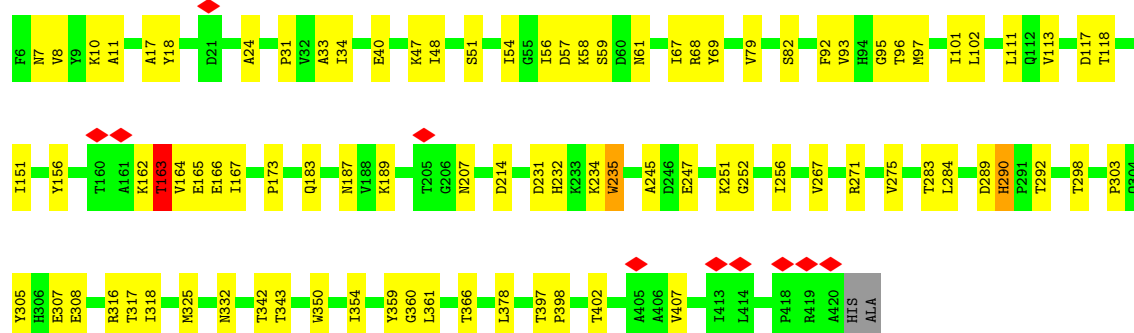
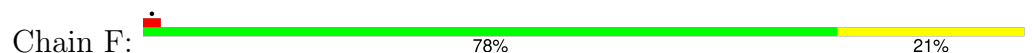
- Molecule 1: Glycoprotein E1



- Molecule 2: Glycoprotein E2




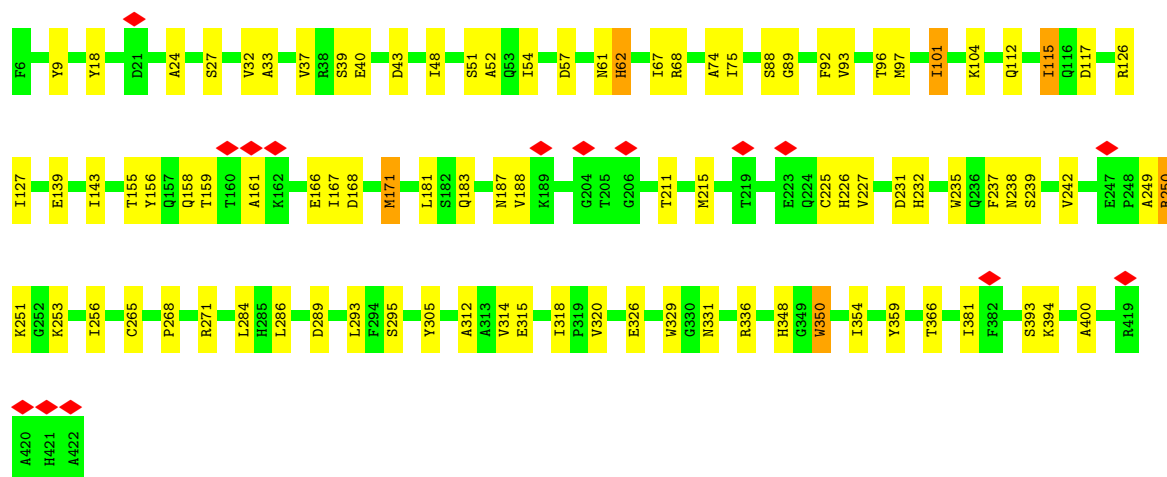
- Molecule 2: Glycoprotein E2




- Molecule 2: Glycoprotein E2

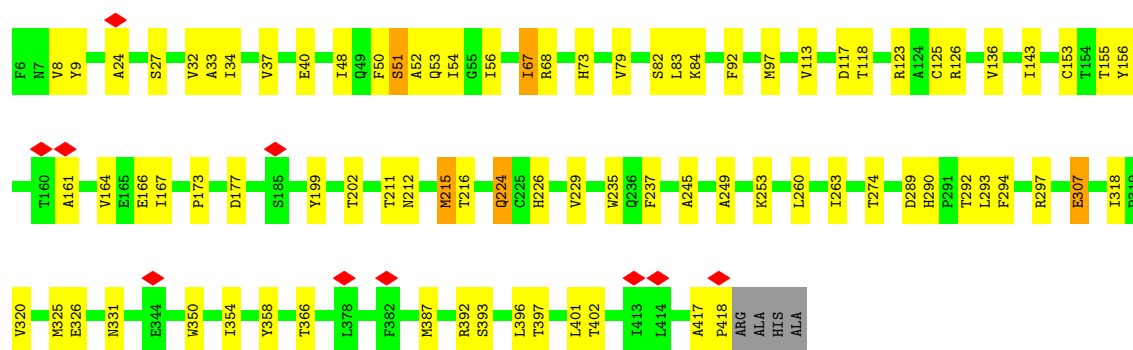


Chain J:  78% 21% .




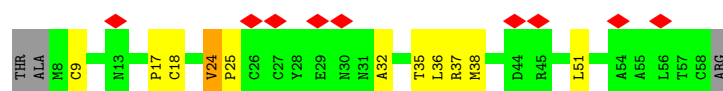
• Molecule 2: Glycoprotein E2

Chain N:  79% 19% ..




• Molecule 3: Assembly protein E3

Chain C:  17% 74% 19% 6% .



• Molecule 3: Assembly protein E3

Chain G:  11% 81% 13% . .

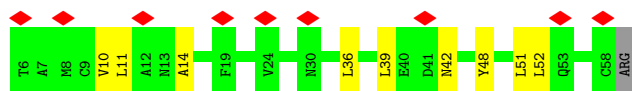
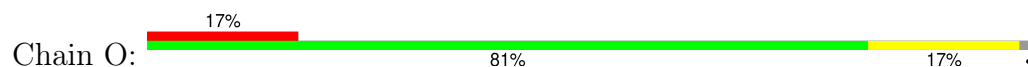


• Molecule 3: Assembly protein E3

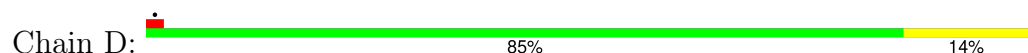
Chain K:  9% 65% 22% 6% . 6%



- Molecule 3: Assembly protein E3



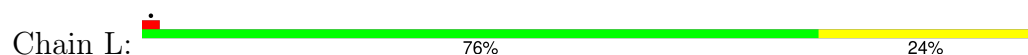
- Molecule 4: Capsid protein



- Molecule 4: Capsid protein



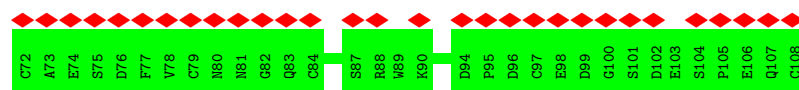
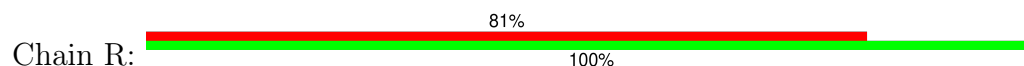
- Molecule 4: Capsid protein



- Molecule 4: Capsid protein



- Molecule 5: Very low-density lipoprotein receptor



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



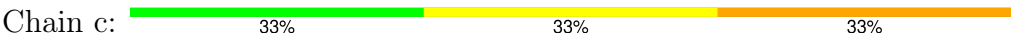
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	439486	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	54.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.794	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	354.75, 354.75, 354.75	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.825, 0.825, 0.825	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.83	5/3415 (0.1%)	0.86	9/4660 (0.2%)
1	E	0.58	0/3415	0.69	0/4660
1	I	0.61	0/3404	0.67	3/4646 (0.1%)
1	M	0.57	0/3404	0.69	1/4646 (0.0%)
2	B	0.54	0/3342	0.69	0/4559
2	F	0.54	0/3326	0.73	1/4537 (0.0%)
2	J	0.55	0/3342	0.70	0/4559
2	N	0.50	0/3310	0.74	1/4516 (0.0%)
3	C	0.37	0/401	0.86	1/549 (0.2%)
3	G	0.40	0/413	0.76	1/563 (0.2%)
3	K	0.48	0/401	1.11	2/549 (0.4%)
3	O	0.37	0/413	0.65	0/566
4	D	0.51	0/1191	0.75	1/1609 (0.1%)
4	H	0.47	0/1199	0.84	2/1620 (0.1%)
4	L	0.50	0/1193	0.67	0/1613
4	P	0.43	0/1199	0.76	0/1620
5	R	0.18	0/280	0.41	0/379
All	All	0.57	5/33648 (0.0%)	0.74	22/45851 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	F	0	1
2	J	0	1
2	N	0	1
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	3
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	PRO	CB-CG	24.63	2.72	1.49
1	A	237	PRO	CG-CD	-16.94	0.93	1.50
1	A	236	THR	C-N	8.31	1.43	1.33
1	A	237	PRO	N-CD	7.84	1.58	1.47
1	A	237	PRO	CA-CB	-6.78	1.43	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	PRO	CB-CG-CD	-28.89	13.64	106.10
1	A	237	PRO	CA-CB-CG	-10.02	85.47	104.50
4	H	143	PRO	CA-N-CD	-9.01	99.39	112.00
1	A	237	PRO	N-CD-CG	-8.43	90.56	103.20
1	A	237	PRO	N-CA-CB	-8.21	93.51	103.45

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	LEU	Peptide
2	B	264	THR	Peptide
3	C	24	VAL	Peptide
2	F	247	GLU	Peptide
2	J	249	ALA	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3329	0	3247	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3329	0	3245	47	0
1	I	3318	0	3232	57	0
1	M	3318	0	3236	51	0
2	B	3249	0	3161	62	0
2	F	3234	0	3149	59	0
2	J	3249	0	3161	70	0
2	N	3218	0	3131	62	0
3	C	392	0	364	9	0
3	G	404	0	376	6	0
3	K	392	0	363	14	0
3	O	404	0	376	6	0
4	D	1163	0	1126	14	0
4	H	1171	0	1137	37	0
4	L	1165	0	1126	27	0
4	P	1171	0	1137	28	0
5	R	275	0	217	0	0
6	Q	28	0	25	1	0
6	U	28	0	25	1	0
6	V	28	0	25	2	0
6	W	28	0	25	1	0
6	X	28	0	25	0	0
6	a	28	0	25	1	0
7	S	39	0	34	0	0
7	T	39	0	34	1	0
7	Y	39	0	34	1	0
7	Z	39	0	34	1	0
7	b	39	0	34	1	0
7	c	39	0	34	1	0
8	G	14	0	13	0	0
8	K	14	0	13	0	0
9	R	1	0	0	0	0
All	All	33212	0	32164	553	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 553 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:CG	1:A:237:PRO:N	1.84	1.39
1:A:237:PRO:CD	1:A:237:PRO:HG3	1.69	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:CG	1:A:237:PRO:HD3	1.60	1.10
1:A:237:PRO:CG	1:A:237:PRO:HD2	1.60	1.10
1:A:237:PRO:CD	1:A:237:PRO:HG2	1.69	1.09

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/438 (100%)	436 (100%)	0	0	100	100
1	E	436/438 (100%)	436 (100%)	0	0	100	100
1	I	435/438 (99%)	434 (100%)	0	1 (0%)	44	72
1	M	435/438 (99%)	434 (100%)	1 (0%)	0	100	100
2	B	415/417 (100%)	409 (99%)	3 (1%)	3 (1%)	19	51
2	F	413/417 (99%)	405 (98%)	4 (1%)	4 (1%)	13	44
2	J	415/417 (100%)	413 (100%)	0	2 (0%)	25	57
2	N	411/417 (99%)	407 (99%)	1 (0%)	3 (1%)	19	51
3	C	49/54 (91%)	46 (94%)	3 (6%)	0	100	100
3	G	50/54 (93%)	49 (98%)	0	1 (2%)	6	34
3	K	49/54 (91%)	44 (90%)	3 (6%)	2 (4%)	2	22
3	O	51/54 (94%)	51 (100%)	0	0	100	100
4	D	150/153 (98%)	150 (100%)	0	0	100	100
4	H	151/153 (99%)	151 (100%)	0	0	100	100
4	L	151/153 (99%)	151 (100%)	0	0	100	100
4	P	151/153 (99%)	150 (99%)	0	1 (1%)	19	51
5	R	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4233/4285 (99%)	4201 (99%)	15 (0%)	17 (0%)	32 62

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	164	VAL
2	B	205	THR
2	F	162	LYS
2	F	163	THR
2	J	250	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	372/372 (100%)	369 (99%)	3 (1%)	79 85
1	E	372/372 (100%)	367 (99%)	5 (1%)	65 77
1	I	371/372 (100%)	365 (98%)	6 (2%)	58 74
1	M	371/372 (100%)	370 (100%)	1 (0%)	91 94
2	B	355/355 (100%)	353 (99%)	2 (1%)	84 90
2	F	354/355 (100%)	348 (98%)	6 (2%)	56 73
2	J	355/355 (100%)	348 (98%)	7 (2%)	50 68
2	N	353/355 (99%)	346 (98%)	7 (2%)	50 68
3	C	44/46 (96%)	44 (100%)	0	100 100
3	G	45/46 (98%)	44 (98%)	1 (2%)	47 65
3	K	44/46 (96%)	43 (98%)	1 (2%)	45 64
3	O	45/46 (98%)	45 (100%)	0	100 100
4	D	122/124 (98%)	121 (99%)	1 (1%)	79 85
4	H	123/124 (99%)	122 (99%)	1 (1%)	79 85
4	L	122/124 (98%)	122 (100%)	0	100 100
4	P	123/124 (99%)	121 (98%)	2 (2%)	58 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	33/33 (100%)	33 (100%)	0	100	100
All	All	3604/3621 (100%)	3561 (99%)	43 (1%)	66	79

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	115	ILE
2	N	51	SER
2	J	171	MET
3	K	24	VAL
2	N	215	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	196	HIS
1	M	9	ASN
2	J	352	HIS
1	M	196	GLN
1	E	139	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	Q	1	1,6	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
6	NAG	Q	2	6	14,14,15	0.23	0	17,19,21	0.50	0
7	NAG	S	1	7,2	14,14,15	0.76	1 (7%)	17,19,21	0.68	0
7	NAG	S	2	7	14,14,15	0.87	1 (7%)	17,19,21	0.55	0
7	BMA	S	3	7	11,11,12	0.56	0	15,15,17	0.91	1 (6%)
7	NAG	T	1	7,2	14,14,15	0.54	0	17,19,21	1.46	2 (11%)
7	NAG	T	2	7	14,14,15	0.57	1 (7%)	17,19,21	0.42	0
7	BMA	T	3	7	11,11,12	0.58	0	15,15,17	0.68	0
6	NAG	U	1	1,6	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
6	NAG	U	2	6	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	V	1	2,6	14,14,15	1.28	1 (7%)	17,19,21	0.72	1 (5%)
6	NAG	V	2	6	14,14,15	0.58	1 (7%)	17,19,21	0.47	0
6	NAG	W	1	2,6	14,14,15	0.33	0	17,19,21	1.67	2 (11%)
6	NAG	W	2	6	14,14,15	0.38	0	17,19,21	0.45	0
6	NAG	X	1	1,6	14,14,15	0.70	0	17,19,21	0.77	0
6	NAG	X	2	6	14,14,15	0.51	0	17,19,21	0.38	0
7	NAG	Y	1	7,2	14,14,15	0.56	0	17,19,21	0.44	0
7	NAG	Y	2	7	14,14,15	0.71	1 (7%)	17,19,21	0.53	0
7	BMA	Y	3	7	11,11,12	0.55	0	15,15,17	0.83	0
7	NAG	Z	1	7,2	14,14,15	0.45	0	17,19,21	1.45	2 (11%)
7	NAG	Z	2	7	14,14,15	0.41	0	17,19,21	0.50	0
7	BMA	Z	3	7	11,11,12	0.62	0	15,15,17	0.66	0
6	NAG	a	1	1,6	14,14,15	0.85	1 (7%)	17,19,21	1.18	1 (5%)
6	NAG	a	2	6	14,14,15	0.49	0	17,19,21	0.37	0
7	NAG	b	1	7,2	14,14,15	0.87	1 (7%)	17,19,21	0.59	0
7	NAG	b	2	7	14,14,15	1.04	1 (7%)	17,19,21	0.57	0
7	BMA	b	3	7	11,11,12	0.56	0	15,15,17	0.85	0
7	NAG	c	1	7,2	14,14,15	0.45	0	17,19,21	1.46	3 (17%)
7	NAG	c	2	7	14,14,15	0.48	0	17,19,21	0.43	0
7	BMA	c	3	7	11,11,12	0.77	1 (9%)	15,15,17	0.76	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	Q	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	S	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	NAG	T	1	7,2	-	6/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	1/6/23/26	0/1/1/1
6	NAG	V	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	V	2	6	-	3/6/23/26	0/1/1/1
6	NAG	W	1	2,6	-	6/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
7	NAG	Y	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Y	3	7	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	7,2	-	5/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	0/2/19/22	0/1/1/1
6	NAG	a	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
7	NAG	b	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	NAG	c	1	7,2	-	6/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1	NAG	O5-C1	-4.50	1.36	1.43
7	b	2	NAG	O5-C1	-3.85	1.37	1.43
7	S	2	NAG	O5-C1	-3.09	1.38	1.43
7	b	1	NAG	O5-C1	-3.04	1.38	1.43
7	Y	2	NAG	O5-C1	-2.52	1.39	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	1	NAG	C2-N2-C7	4.69	129.19	122.90
6	W	1	NAG	C2-N2-C7	4.63	129.11	122.90
7	Z	1	NAG	C2-N2-C7	4.63	129.11	122.90
7	c	1	NAG	C2-N2-C7	4.48	128.91	122.90
6	U	1	NAG	C1-O5-C5	3.37	116.71	112.19

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	1	NAG	C4-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
7	c	2	NAG	C4-C5-C6-O6

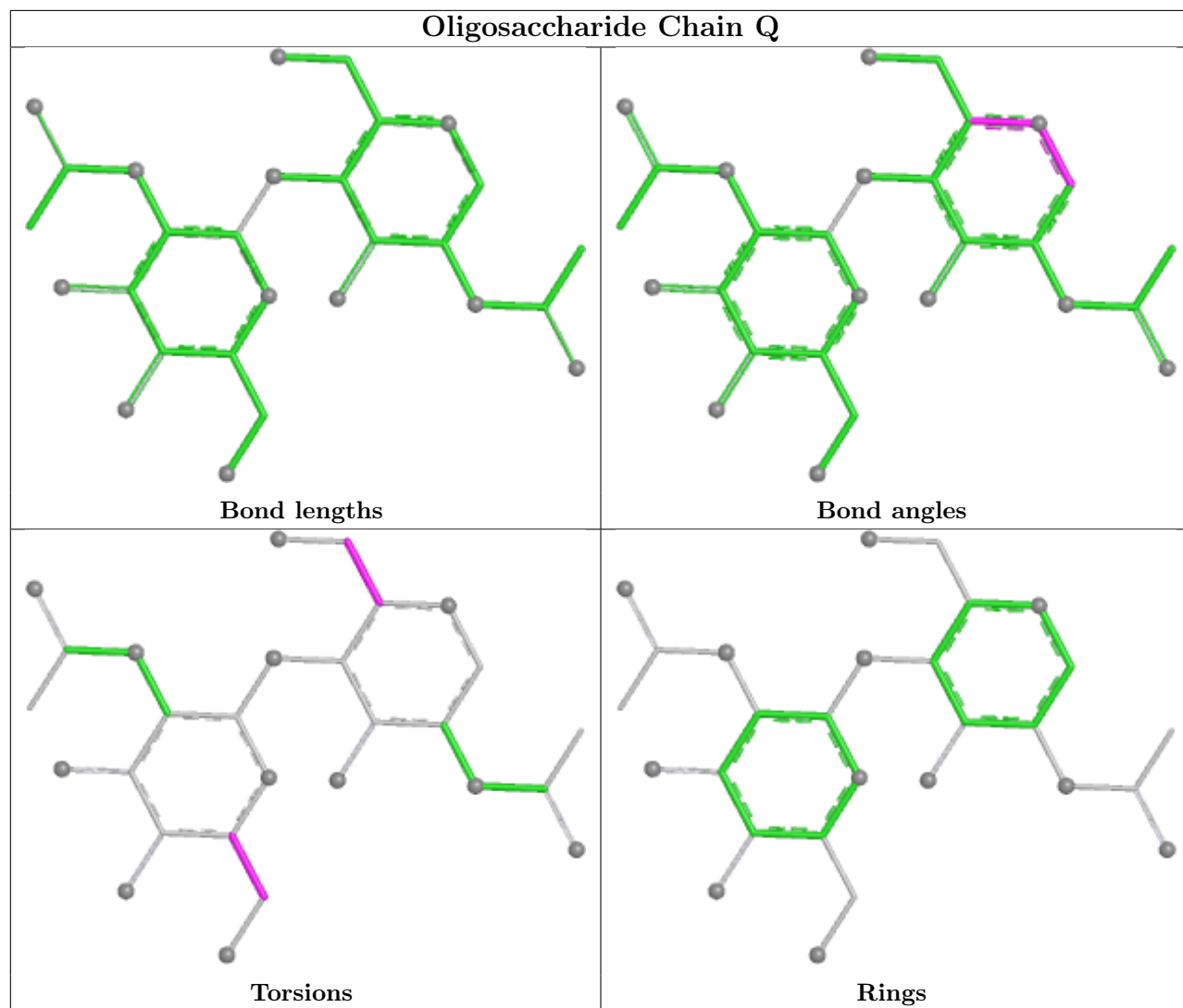
There are no ring outliers.

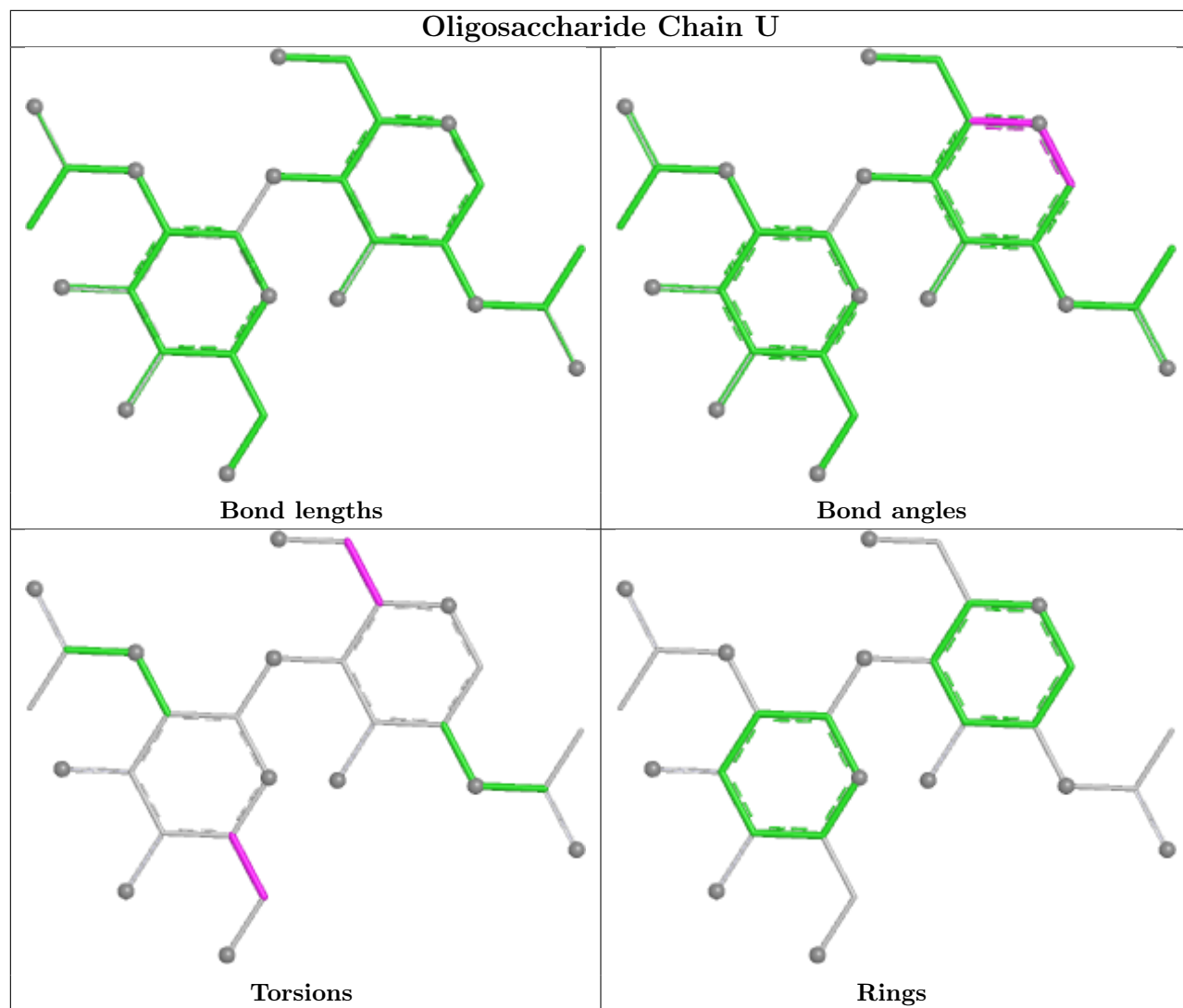
14 monomers are involved in 11 short contacts:

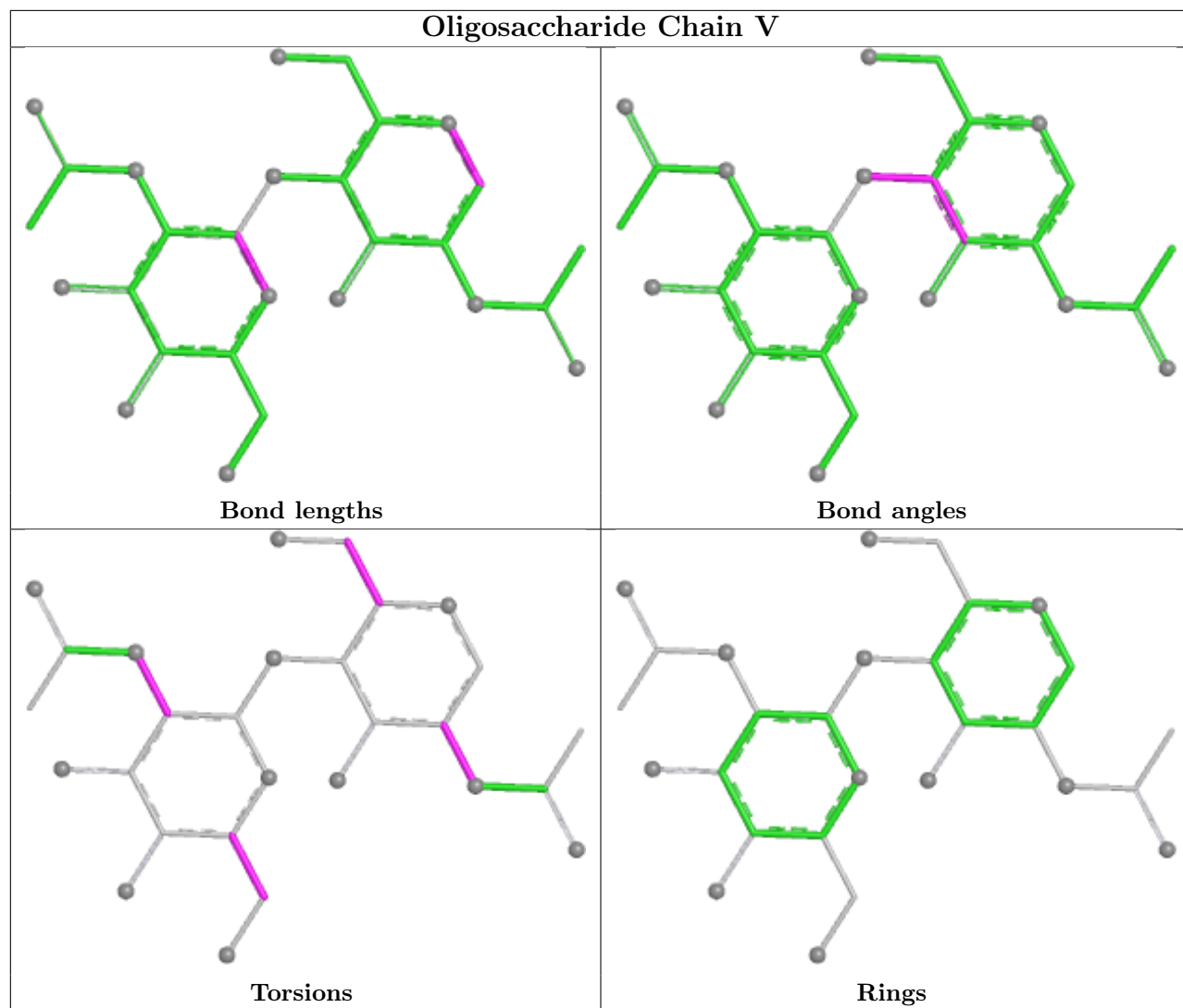
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	2	NAG	1	0
7	Z	1	NAG	1	0
7	b	1	NAG	1	0
6	V	1	NAG	1	0
6	W	1	NAG	1	0
6	V	2	NAG	1	0
6	U	1	NAG	1	0
7	T	1	NAG	1	0
6	a	1	NAG	1	0
7	Y	1	NAG	1	0
7	b	2	NAG	1	0
7	Y	2	NAG	1	0
7	c	1	NAG	1	0
6	Q	1	NAG	1	0

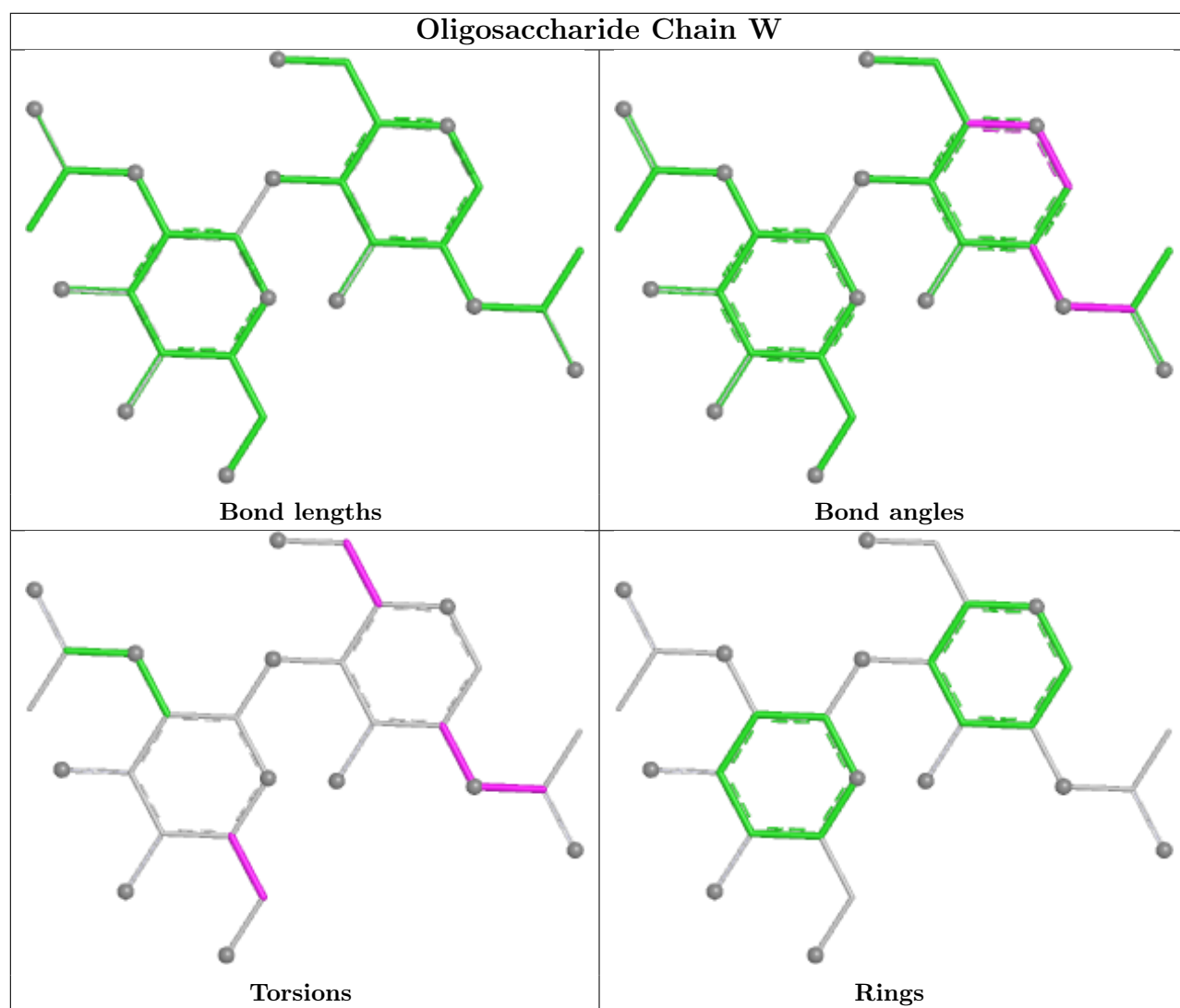
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

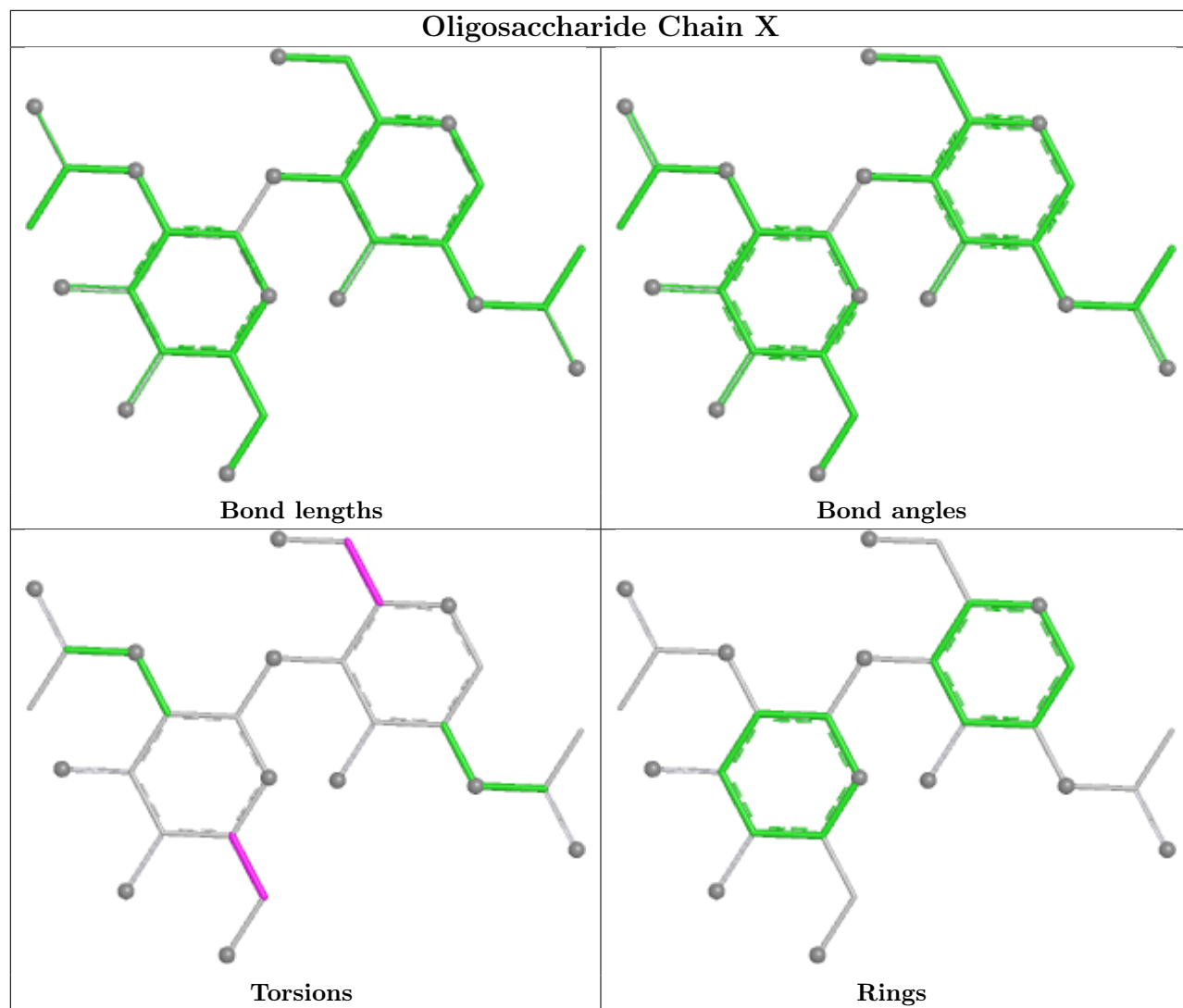


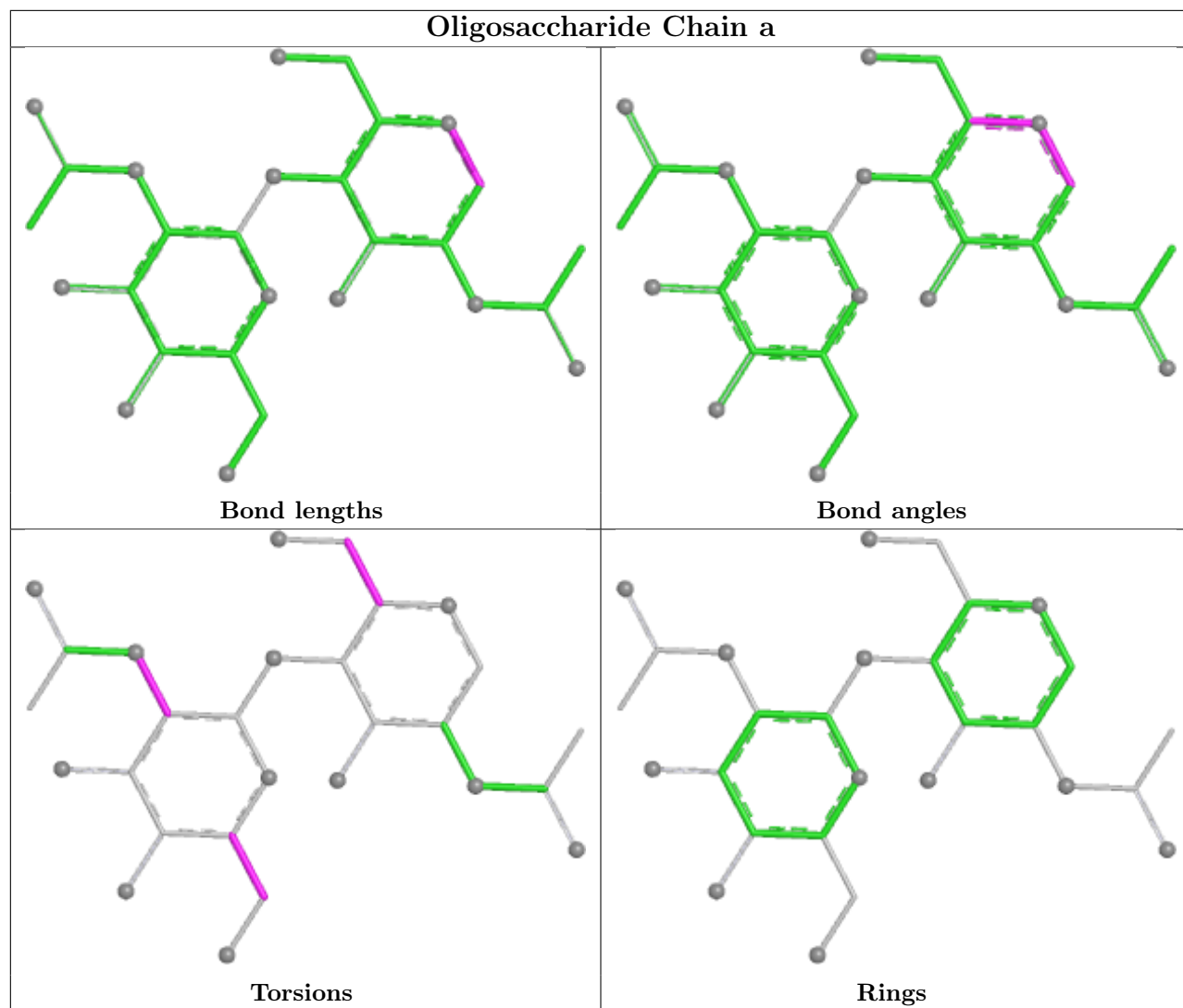


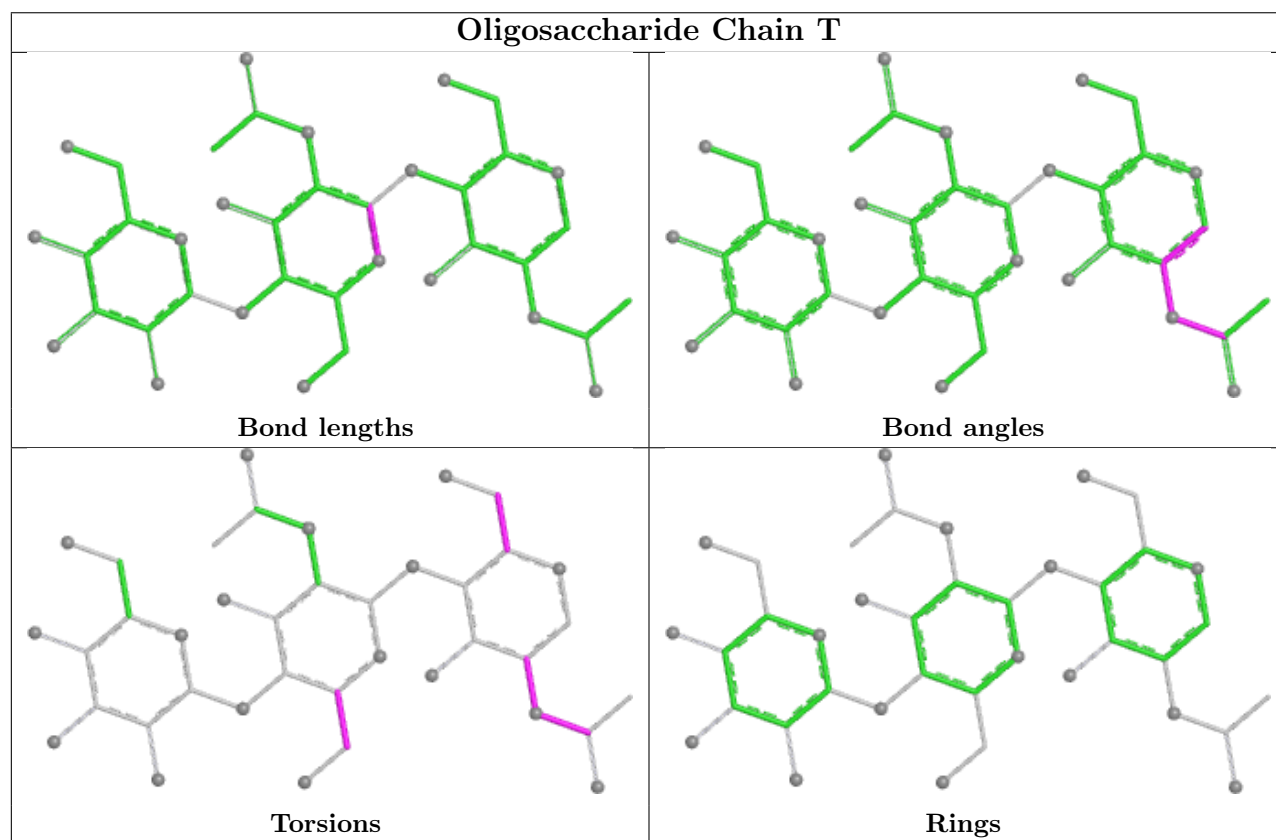
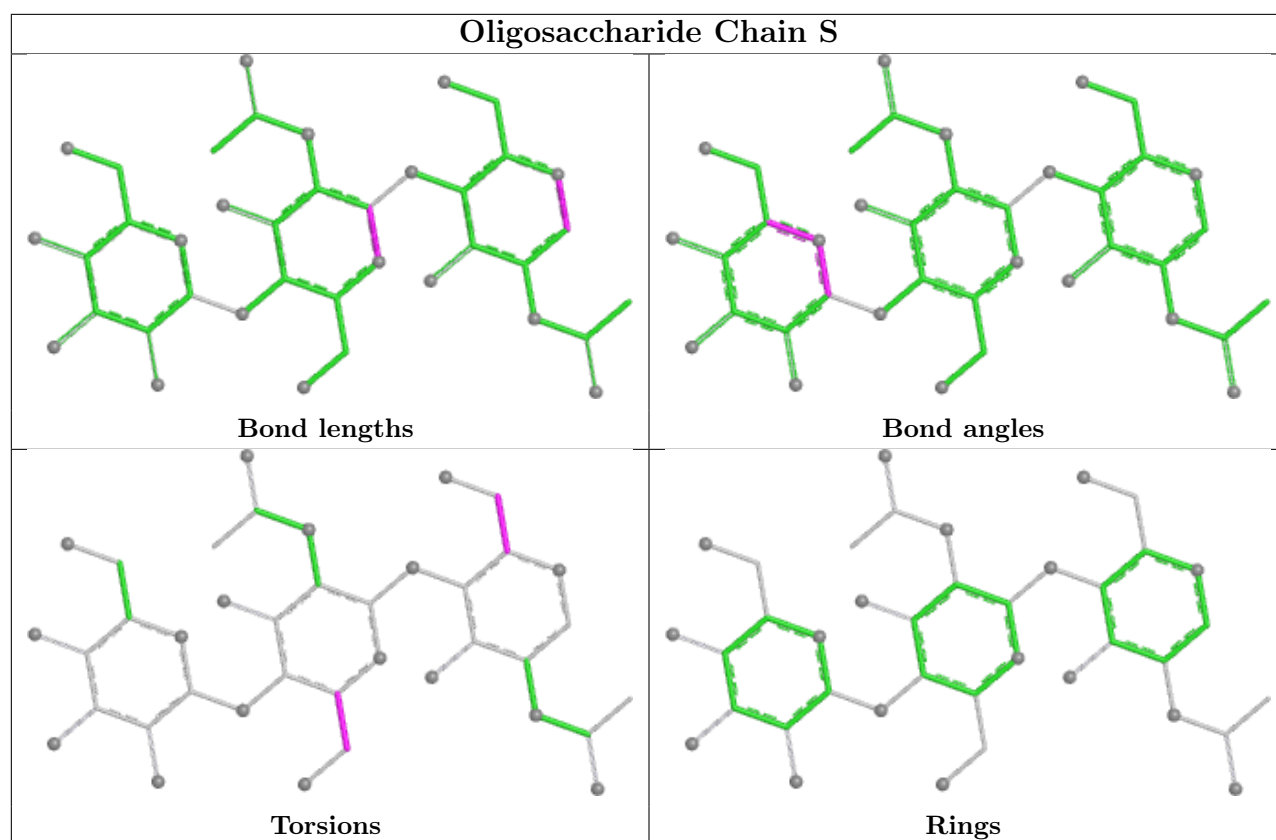


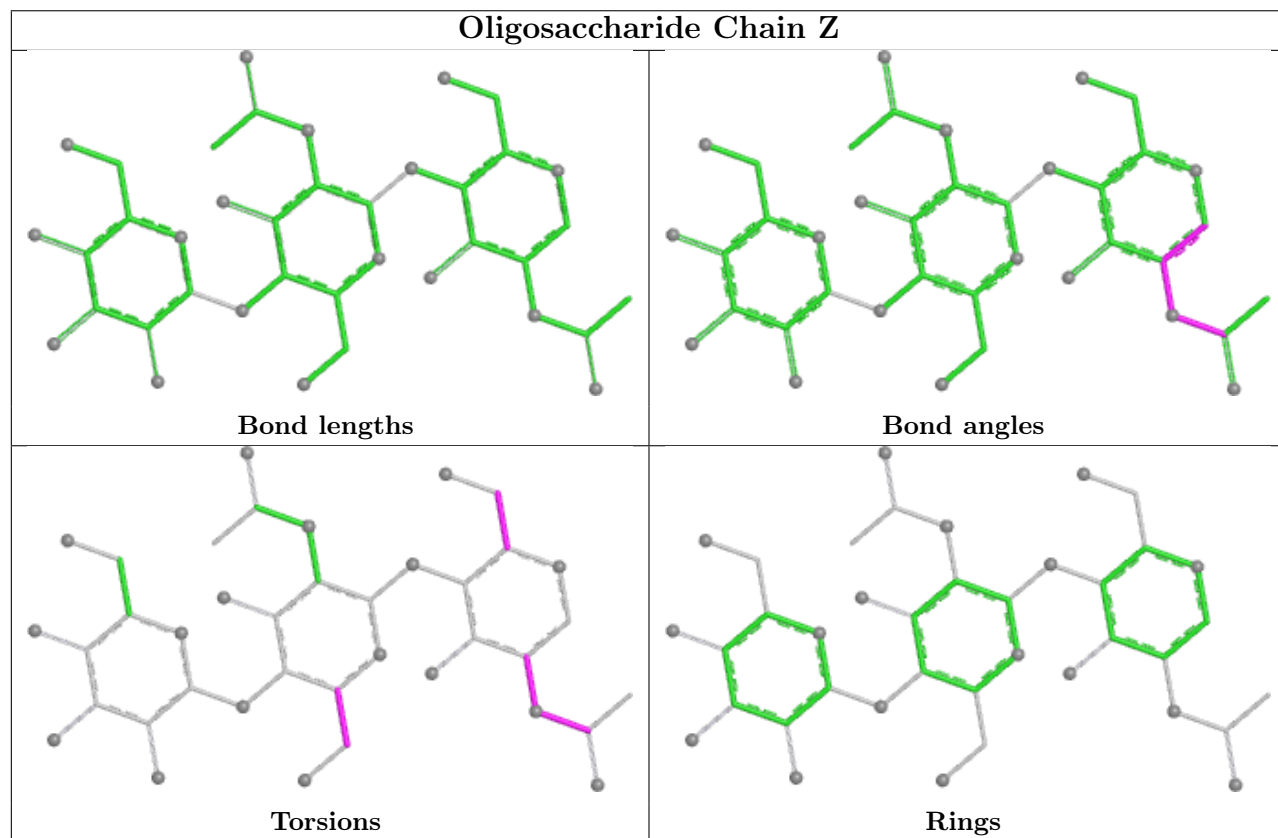
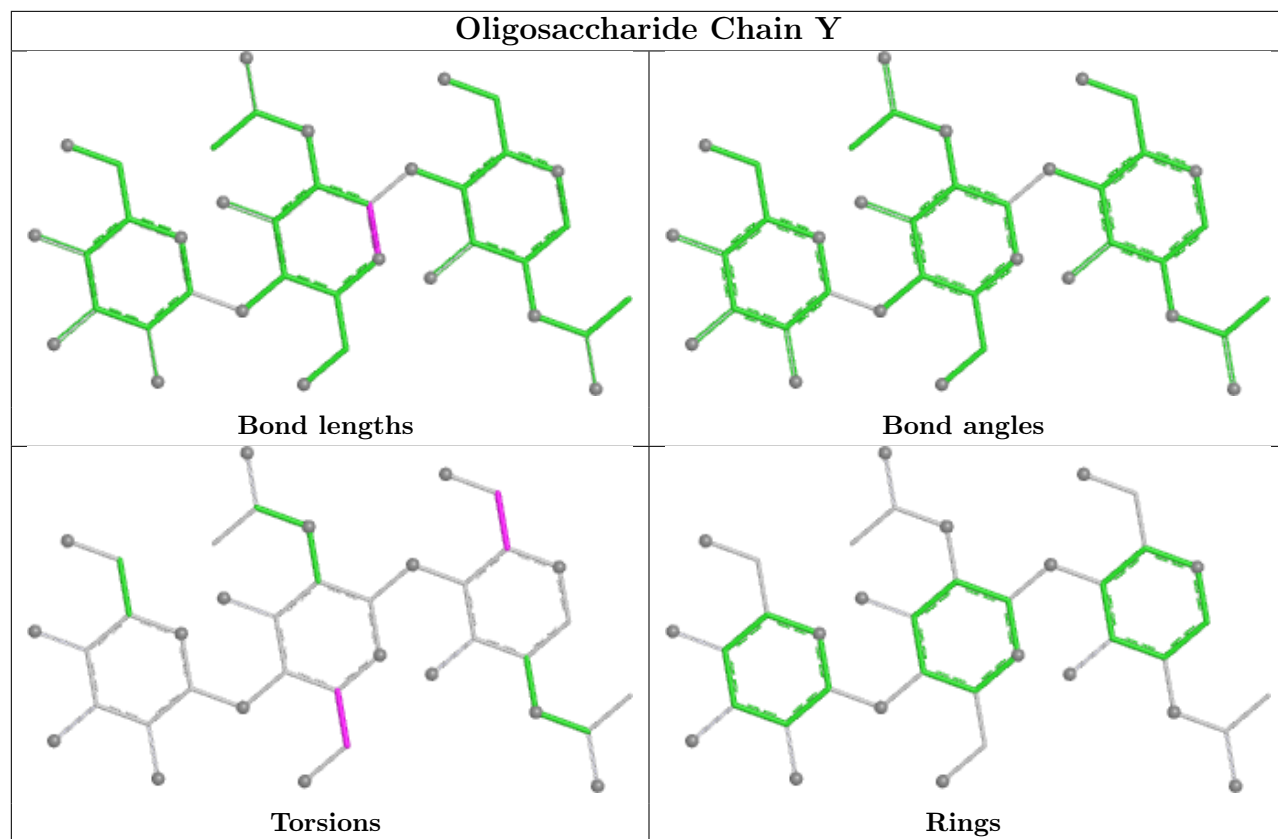




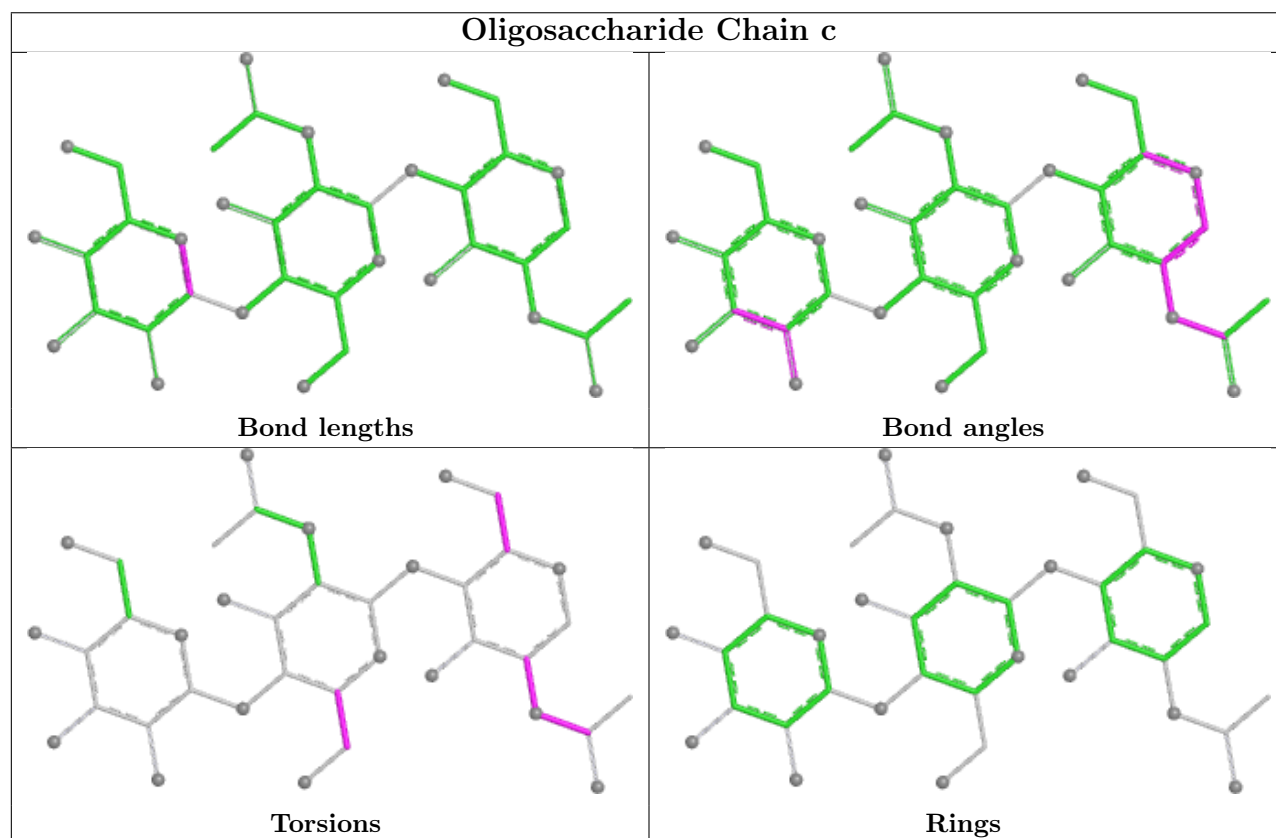
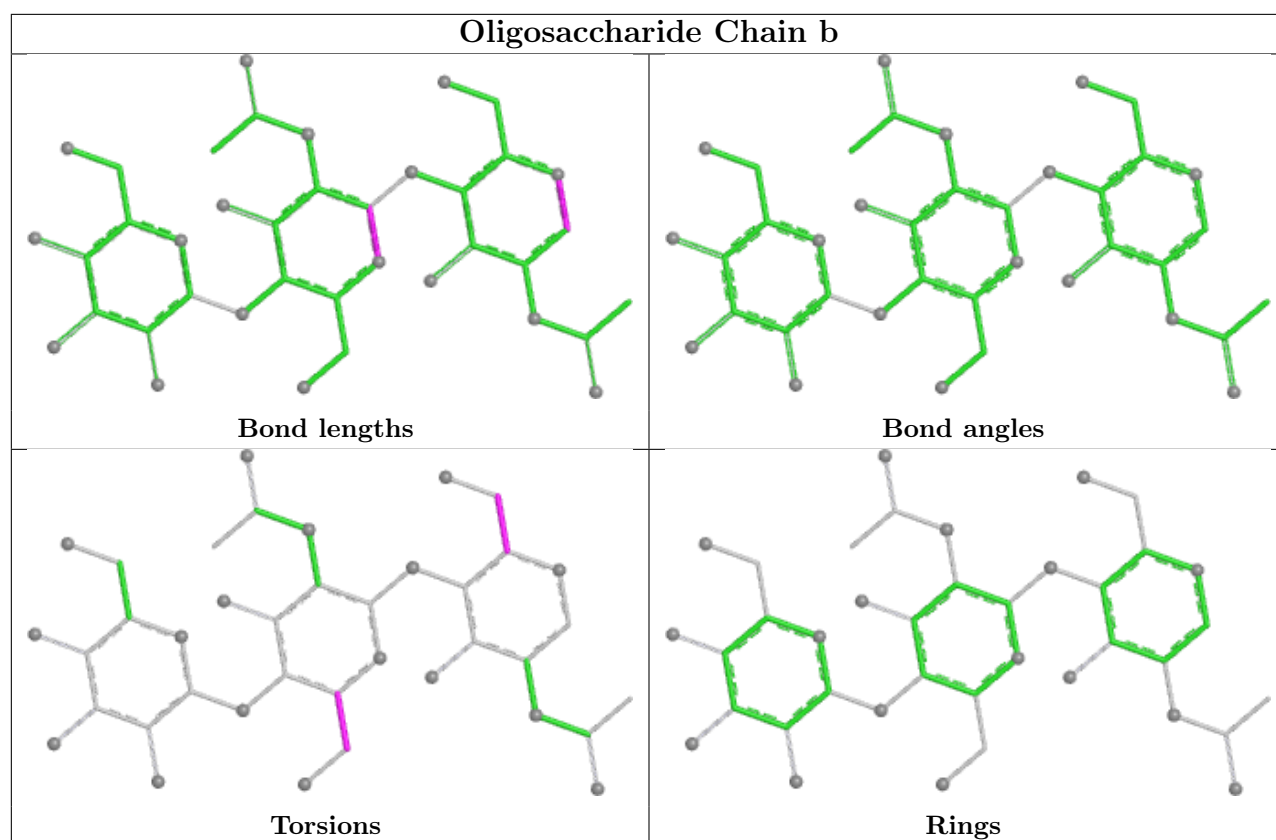












## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NAG	K	101	3	14,14,15	0.24	0	17,19,21	0.34	0
8	NAG	G	101	3	14,14,15	0.25	0	17,19,21	0.60	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	K	101	3	-	1/6/23/26	0/1/1/1
8	NAG	G	101	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	101	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

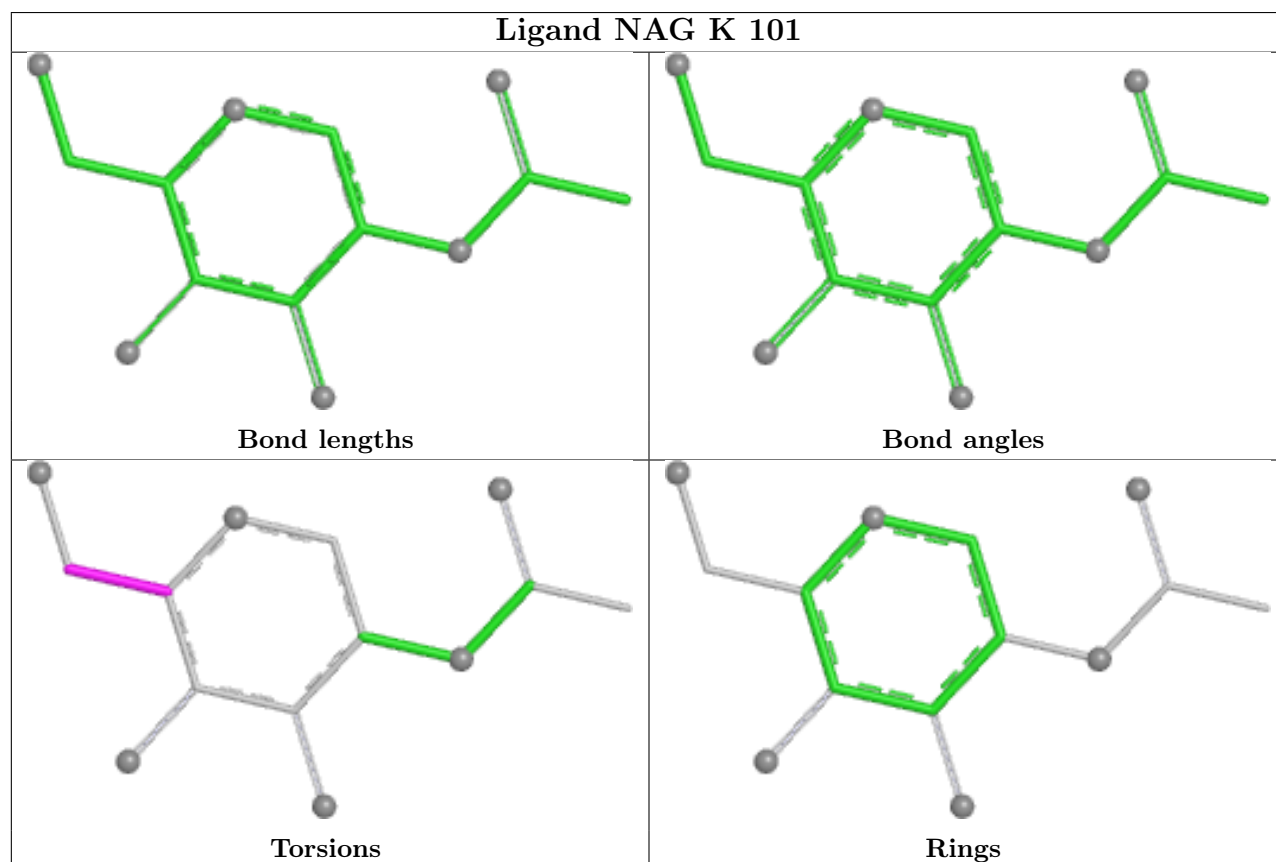
Mol	Chain	Res	Type	Atoms
8	G	101	NAG	C4-C5-C6-O6
8	G	101	NAG	O5-C5-C6-O6
8	K	101	NAG	O5-C5-C6-O6

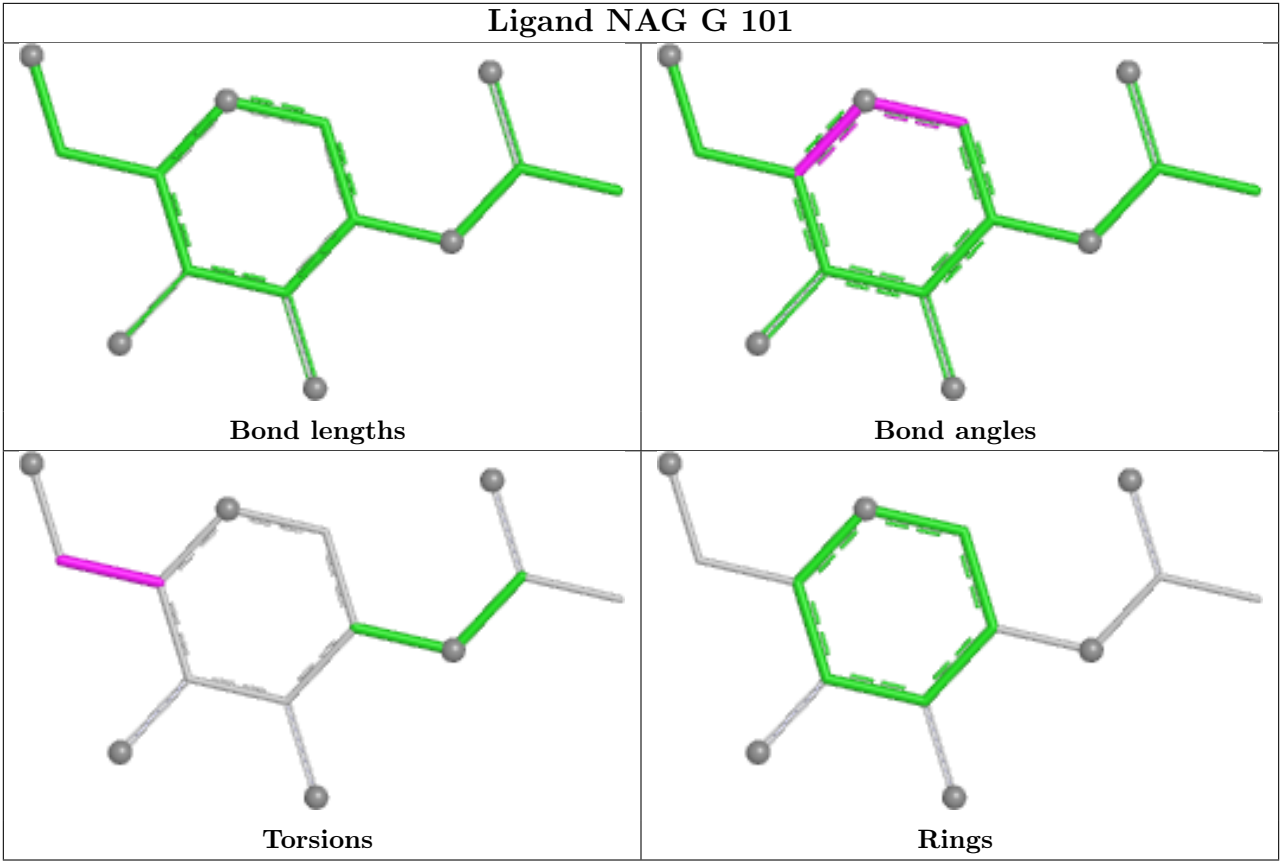
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	29:HIS	C	30:SER	N	1.20

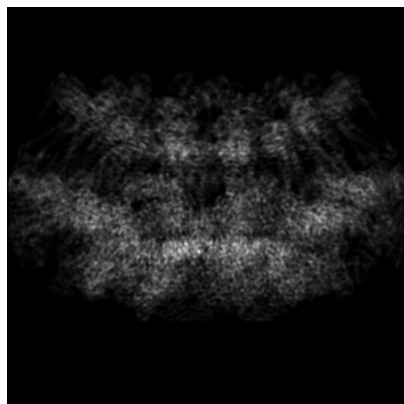
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42054. These allow visual inspection of the internal detail of the map and identification of artifacts.

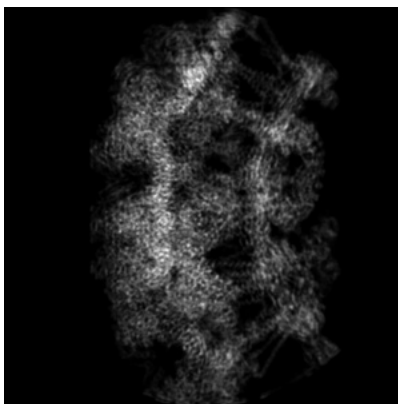
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

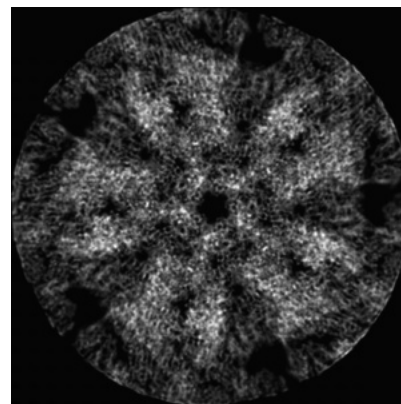
#### 6.1.1 Primary map



X

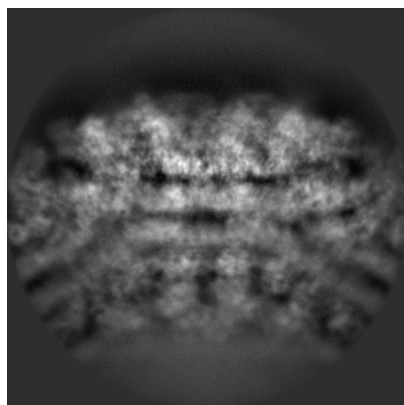


Y

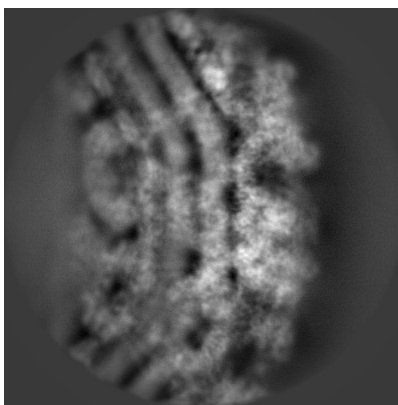


Z

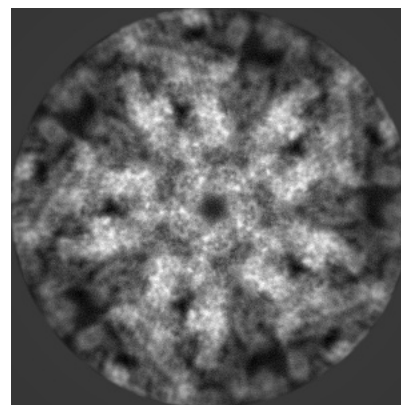
#### 6.1.2 Raw map



X



Y

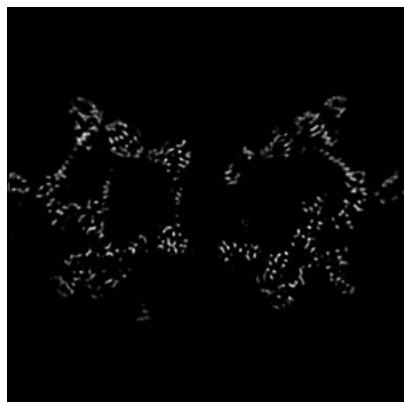


Z

The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

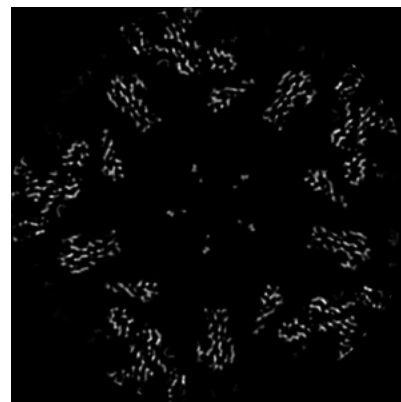
### 6.2.1 Primary map



X Index: 215

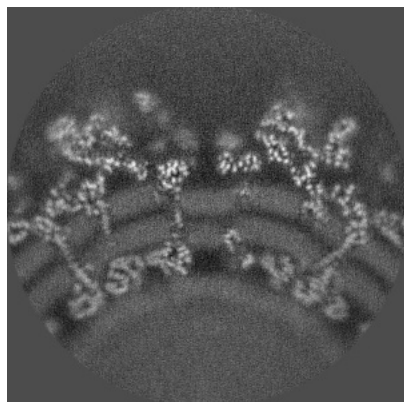


Y Index: 215

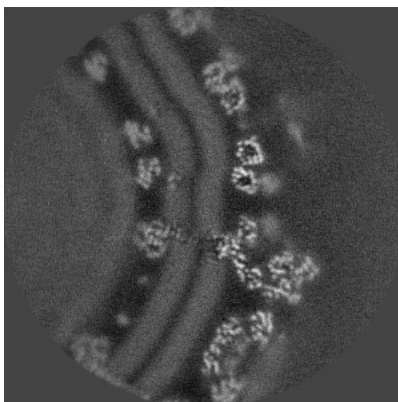


Z Index: 215

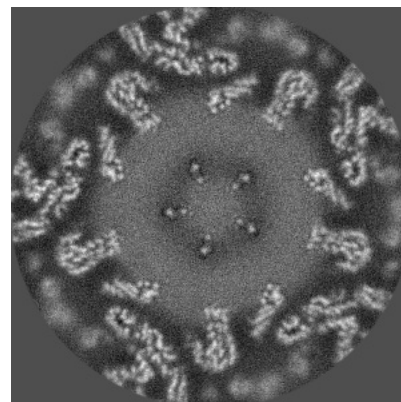
### 6.2.2 Raw map



X Index: 215



Y Index: 215



Z Index: 215

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

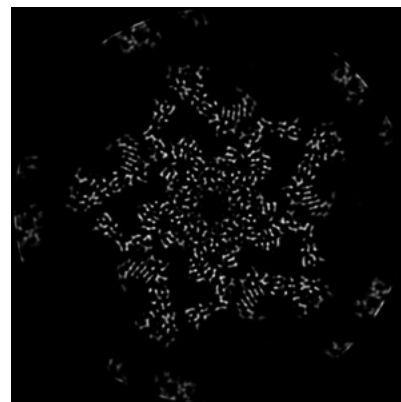
### 6.3.1 Primary map



X Index: 197

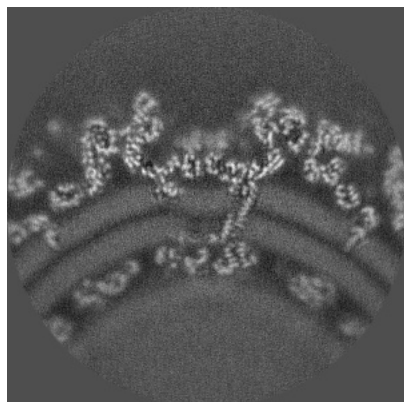


Y Index: 243

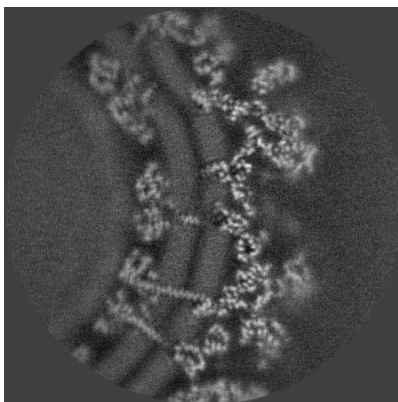


Z Index: 175

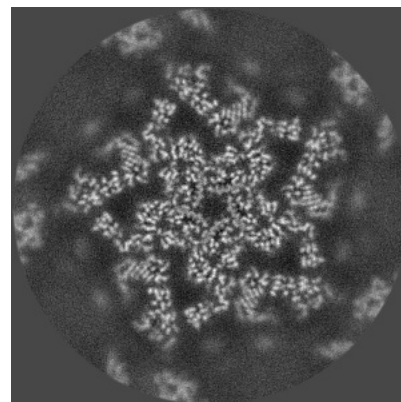
### 6.3.2 Raw map



X Index: 198



Y Index: 250



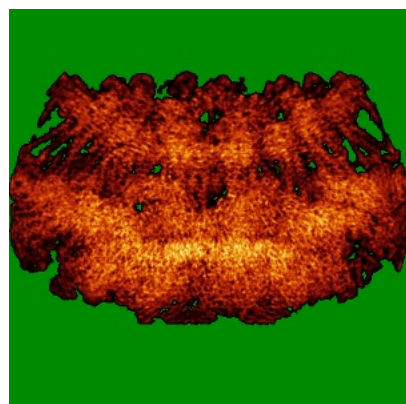
Z Index: 254

The images above show the largest variance slices of the map in three orthogonal directions.

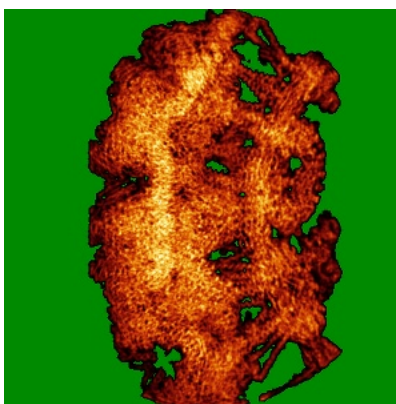


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

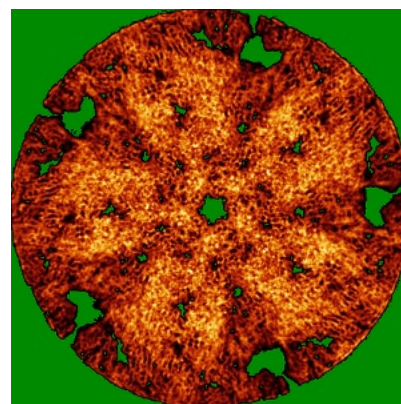
### 6.4.1 Primary map



X

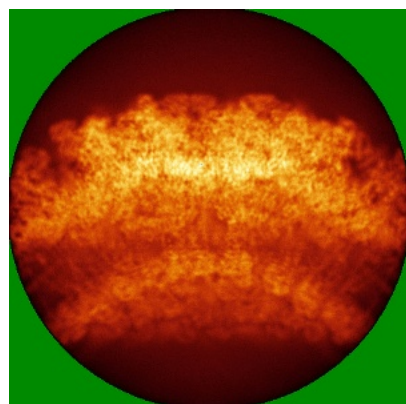


Y

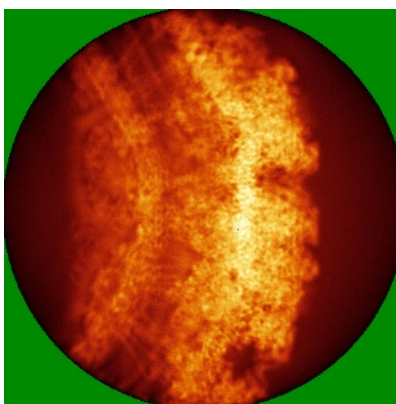


Z

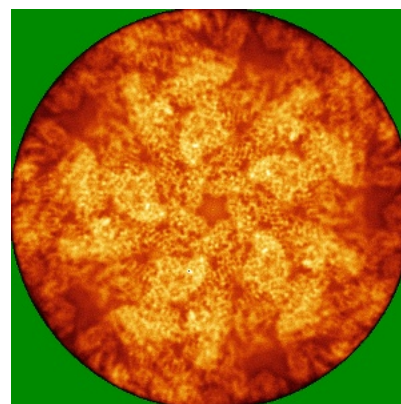
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



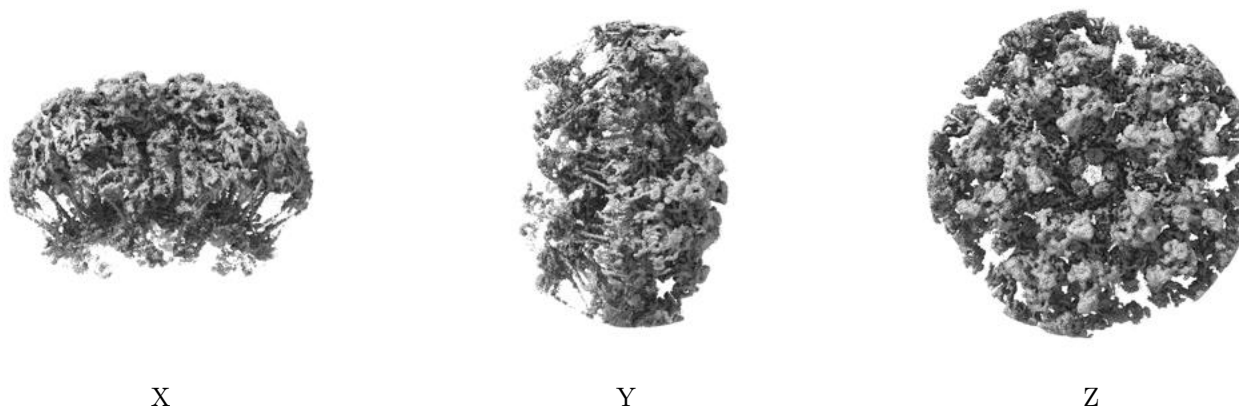
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

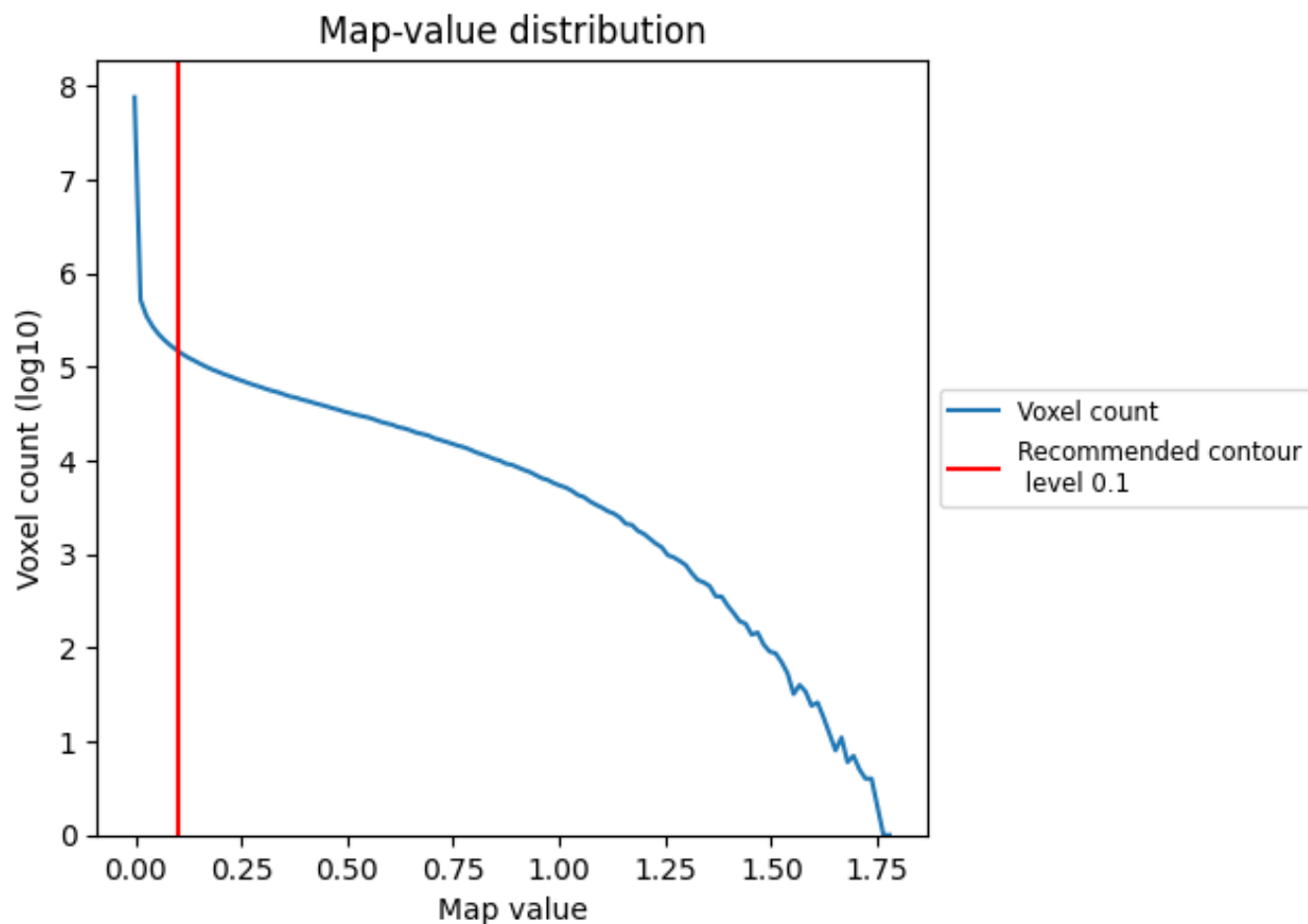
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

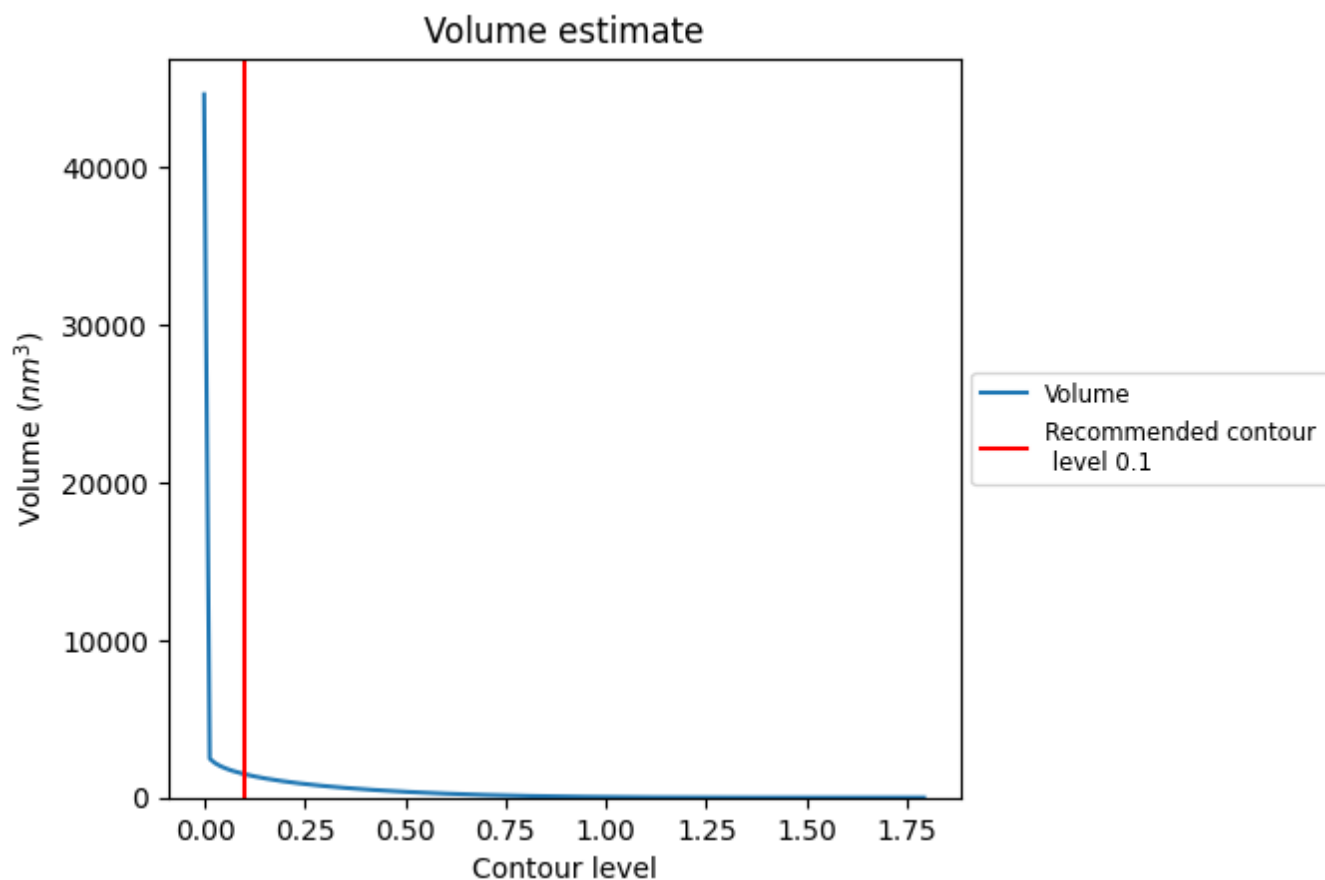
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

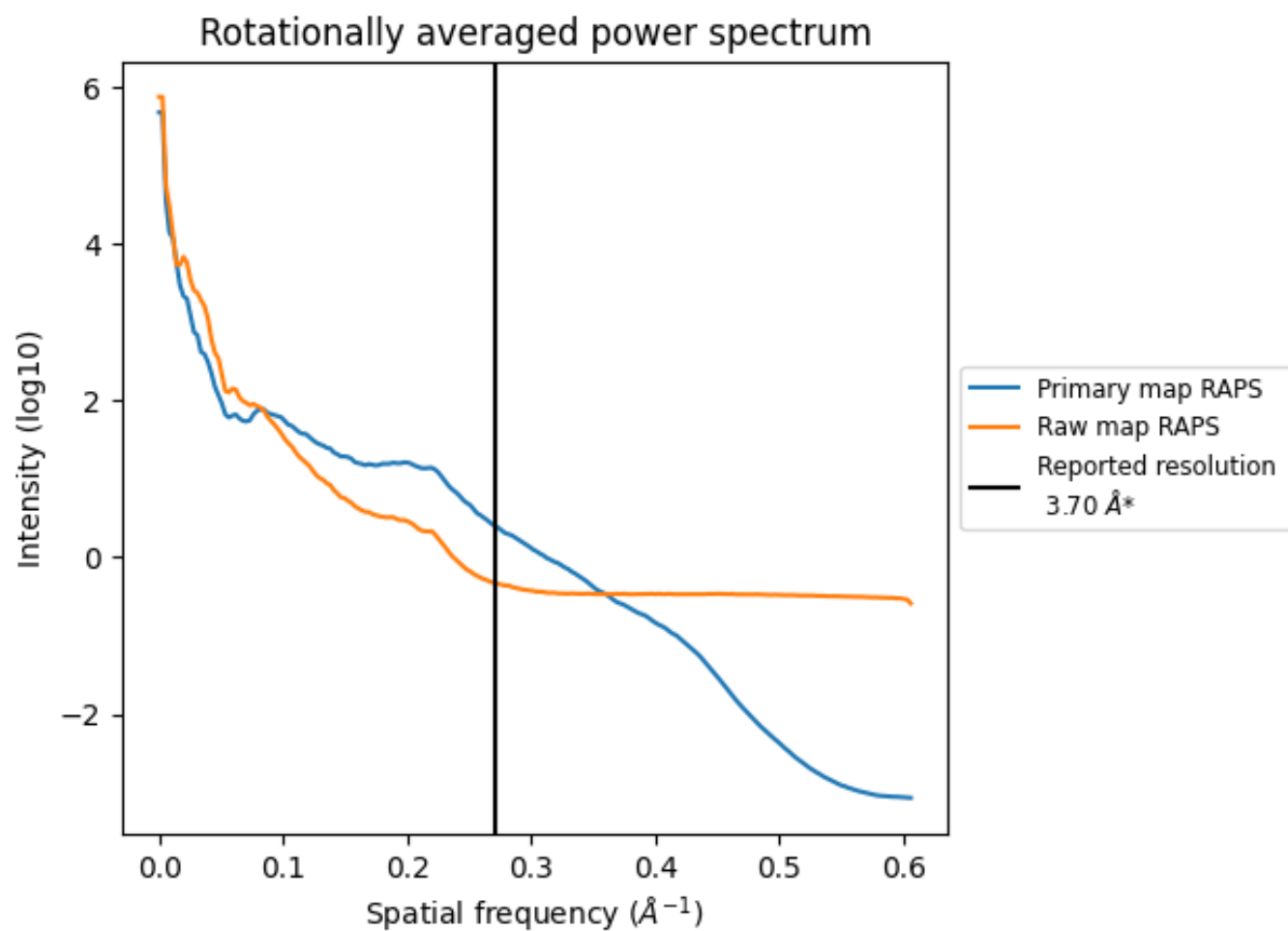
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1480 \text{ nm}^3$ ; this corresponds to an approximate mass of 1337 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

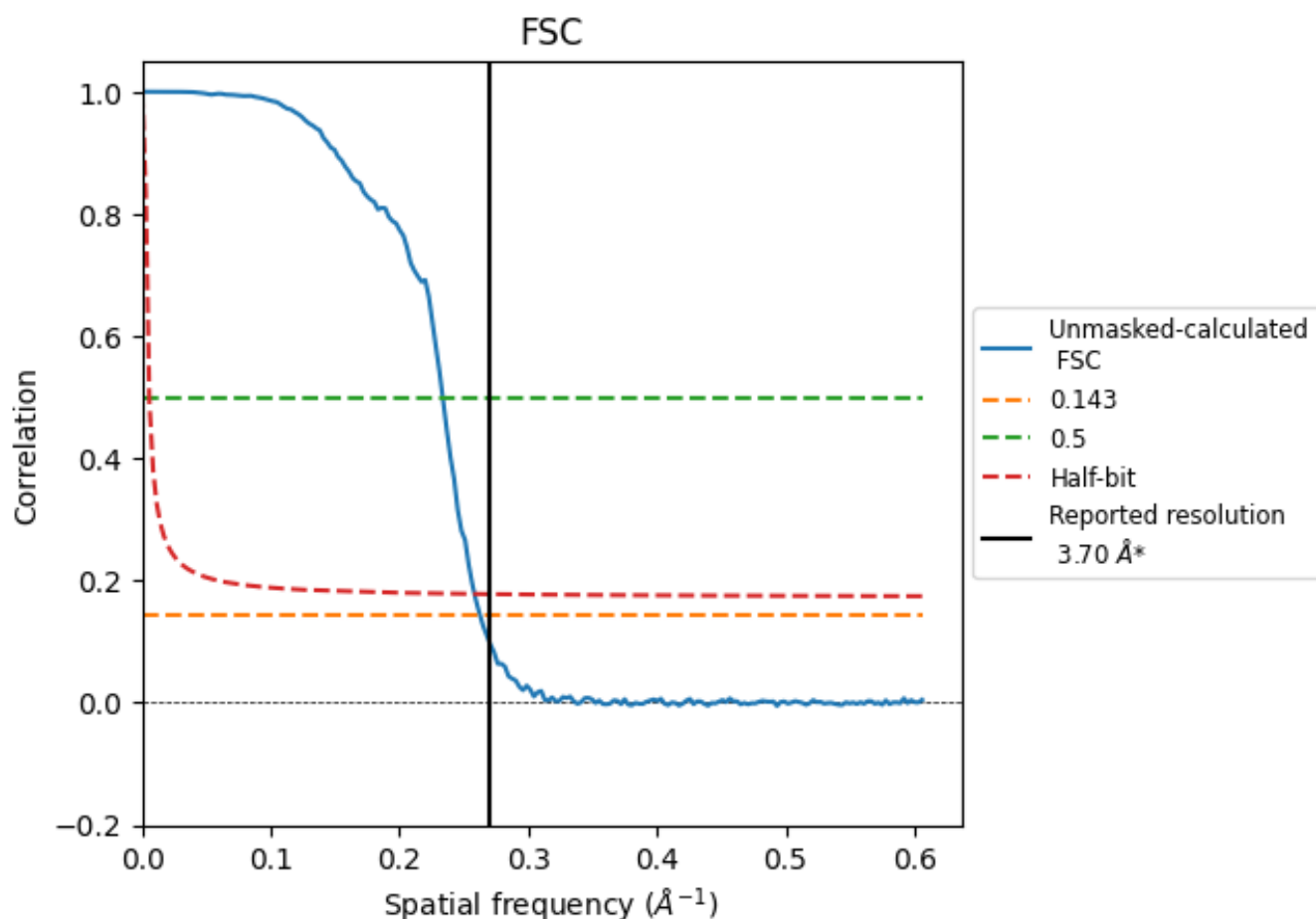


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

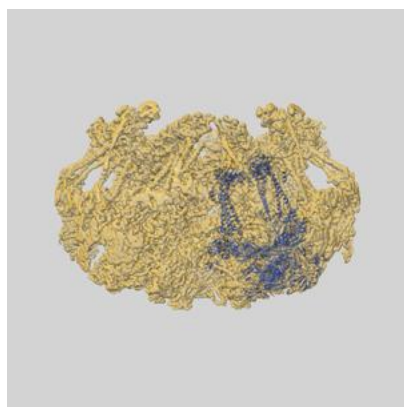
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	4.28	3.87

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

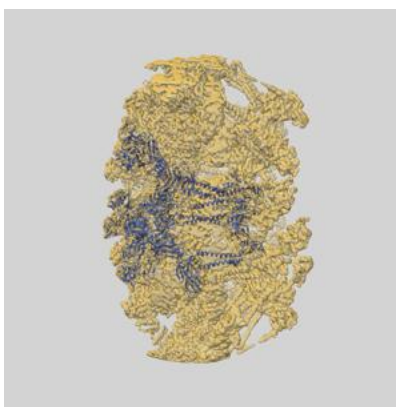
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42054 and PDB model 8UA8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

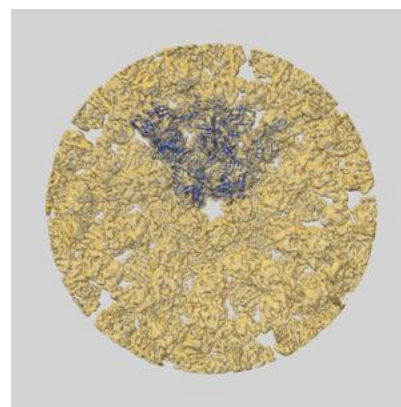
### 9.1 Map-model overlay [i](#)



X



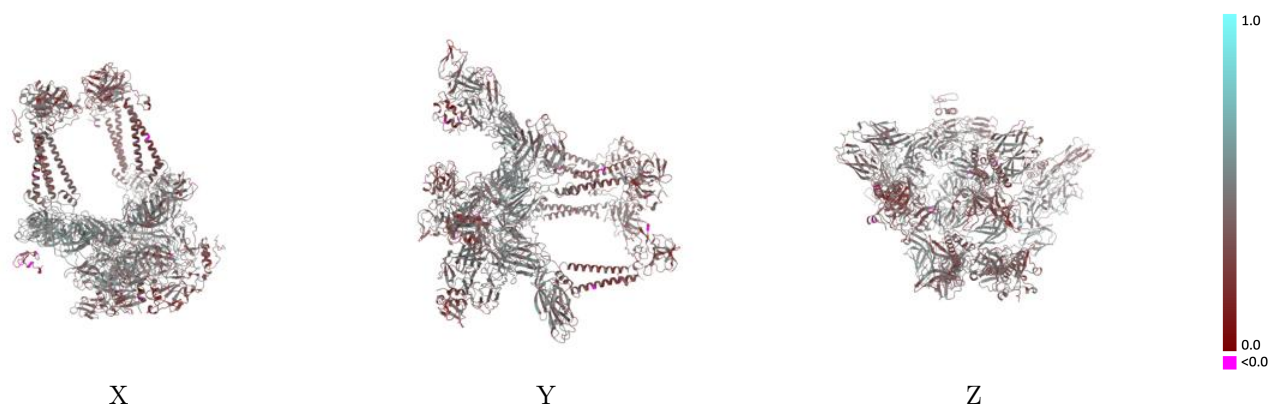
Y



Z

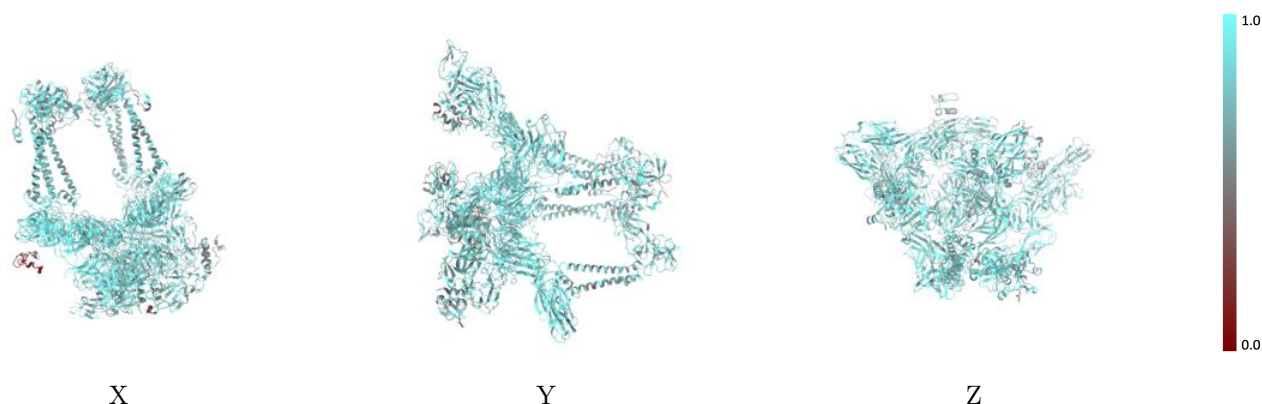
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

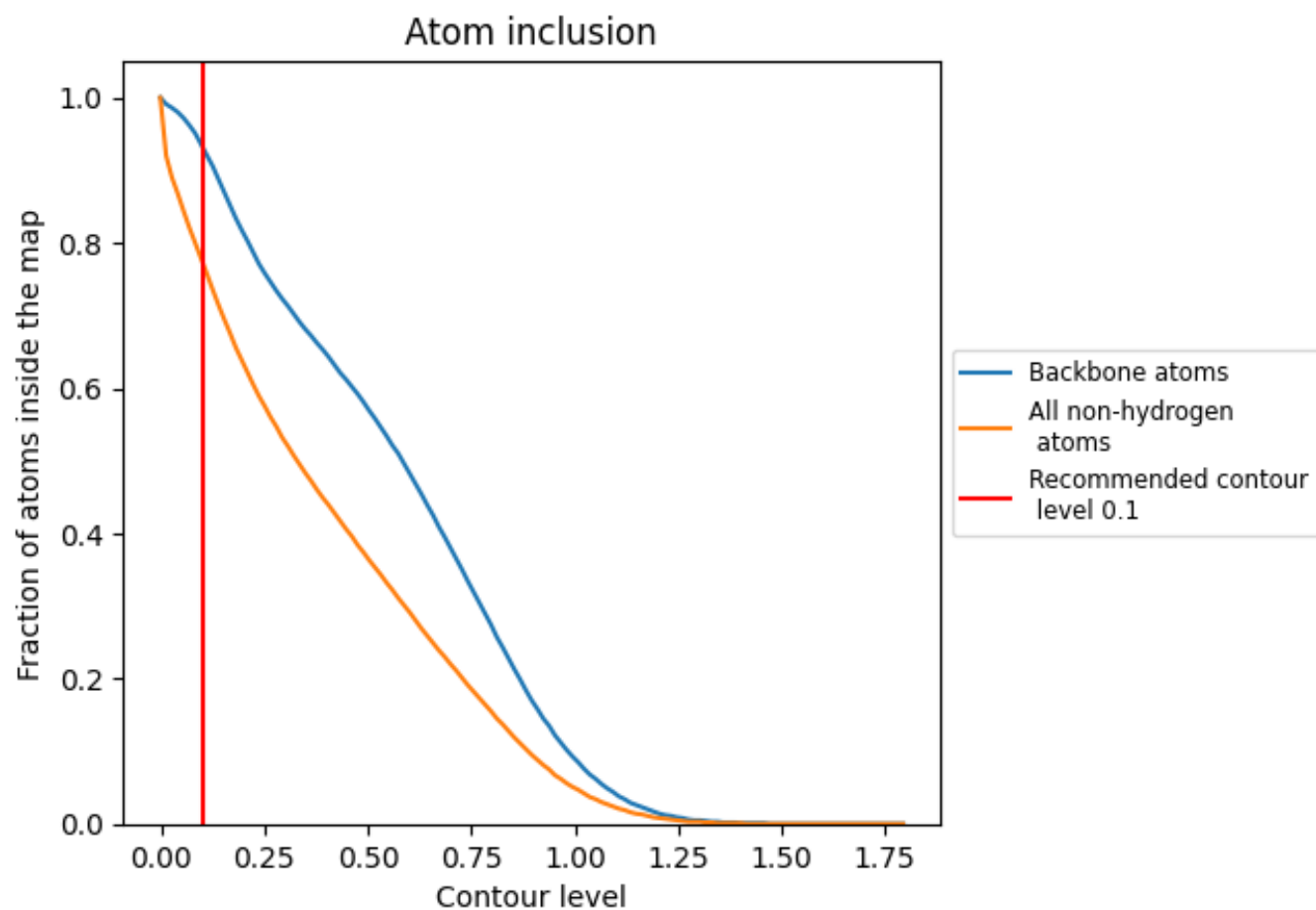
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.4040
A	 0.8220	 0.4460
B	 0.7770	 0.4220
C	 0.5970	 0.2930
D	 0.7690	 0.3730
E	 0.8120	 0.4280
F	 0.7910	 0.4210
G	 0.6140	 0.3060
H	 0.7290	 0.3140
I	 0.8350	 0.4550
J	 0.7710	 0.4170
K	 0.6140	 0.2680
L	 0.7580	 0.3740
M	 0.8140	 0.4220
N	 0.7650	 0.3990
O	 0.5690	 0.2820
P	 0.7270	 0.3160
Q	 0.7140	 0.3960
R	 0.1540	 0.0710
S	 0.4870	 0.2610
T	 0.4870	 0.3570
U	 0.4640	 0.2790
V	 0.7860	 0.5090
W	 0.4640	 0.2410
X	 0.7140	 0.3900
Y	 0.4870	 0.2920
Z	 0.6410	 0.3700
a	 0.6070	 0.2580
b	 0.4620	 0.3720
c	 0.6670	 0.3760

